

# CURRICULUM VITÆ

Angel Rubio Secades

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## I. DATOS DE IDENTIFICACIÓN PERSONAL

Nombre y Apellidos : Angel Rubio Secades  
DNI N° : 9294488-G  
Fecha y Lugar de Nacimiento : 27-Septiembre-1965. Oviedo.  
Domicilio : Paseo Pio Baroja 20, 4B, E-20008 San Sebastián/Donostia  
Teléfonos : Parti.: (34)-9434224033, (móvil: (34)-609811125)  
Dpto. : (34)-943018292  
E-Mail : angel.rubio@mpsd.mpg.de and angel.rubio@ehu.es  
Situación Actual : Scientific Member and Managing Director  
Max Planck Institute for the Structure and Dynamics of Matter (MPSD).  
Luruper Chaussee 149, 22761 Hamburg, Germany:  
Desde 1-Diciembre-2014  
  
Distinguish Research Scientist  
Center for Computational Quantum Physics (CCQ) at the Simons Foundation's Flatiron  
160 Fifth Avenue New York, NY 10010  
Desde 28-Septiembre-2017  
  
Distinguish Professor: Condensed Matter Physics  
Dpto. Física de Materiales, Facultad Químicas. Universidad del País Vasco.  
Nº Registro de Personal : 0929448802 A0500  
Desde 1-Diciembre-2015

## II. TÍTULOS ACADÉMICOS

- *Licenciado en Ciencias Físicas* con “MATRÍCULA DE HONOR”  
Universidad de Valladolid. Junio 1988.
- *Examen de Grado de Licenciatura en Ciencias Físicas* con “MATRÍCULA DE HONOR”  
Tesina: “*Aproximación No-Local al Potencial de Intercambio y Correlación en la Teoría Kohn-Sham. Aplicaciones a Átomos, Clusters y Sólidos*”  
Universidad de Valladolid. 13-Julio-1988.
- *Cursos de Doctorado: “Física Teórica, Física Atómica y Molecular” (1988-1990)*  
Departamento de Física Teórica, Atómica, Molecular y Nuclear  
Universidad de Valladolid.
- *Doctor en Ciencias Físicas* con “SUMMA CUM LAUDE”  
Tesis: “*Estructura Electrónica y Propiedades Ópticas de Agregados Metálicos en la Teoría del Funcional de la Densidad*”  
Universidad de Valladolid. 17-Septiembre-1991.

### III. HONORES

- Fellow of the European Academy of Sciences 2020
- 2018 Max Born Medal and Prize
- Medalla de la Real Sociedad Española de Física (RSEF), Madrid, Diciembre 2016
- Member of the Academia Europaea (May-2016-)
- European Research Council (ERC) Advanced Grant (2016-2021) (QSpec-NewMat)
- XV Manuel Laborde Werlinden Prize for the best technology-based business initiative based on innovative ideas: "Materials Evolution", 2015,
- Premio Jaime I de Investigación Básica 2014.
- Foreign Associate of the U.S. National Academy of Sciences (2014)
- Enbaxadore Honorario Donostia-San Sebastián, "San Sebastián Turismo % Convencion Bureau and Kursaal" (November 2012-)
- External Scientific Member of the Fritz-Haber-Institute of the Max-Planck-Gesellschaft, (Nov. 2011-)
- European Research Council (ERC) Advanced Grant (2011-2016) (DYNamo)
- Fellow of American Association for Advanced Science (AAAS) Physics Section (2010)
- *Distinguished Visiting Scientist*, Fritz Haber Institute der Max-Planck-Gesellschaft, Berlin (2009-2011)
- *Outstanding Referee*, American Physical Society (2009)
- *XVI Premio DuPont de la Ciencia: Nanotecnología*, Dupont Foundation (2006)
- *2005 Friedrich Wilhelm Bessel Research Award*, Humboldt Foundation, Germany
- *2004 Fellow of the American Physical Society: Materials Science Division*
- *2004 Sir Allan Sewell Fellowship*  
School of Science, Griffith University, Australia
- *2001 JSPS Invitation Fellowship Programs for Research in Japan*
- *Becario Postdoctoral FULBRIGHT/MEC*  
Convocatoria: B.O.E. 31-Marzo-1992. (Octubre 1992 - Septiembre 1994)
- Who's Who in the World, 16th Edition (1999); International Who's Who of Professionals, Edition (1999-to date). Who's Who Among Executives and Professionals, 2008-2009 "Honors Edition".
- *Premio Nacional "Jóvenes Investigadores" de la Real Sociedad Española de Física*  
Madrid, Julio 1992.
- *Premio Extraordinario de Doctorado en Ciencias Físicas*  
Facultad de Ciencias. Universidad de Valladolid. Junio 1992.
- *Becario del Programa Sectorial de Formación de Profesorado y Personal Investigador, Subprograma General, (B.O.E. 5-Enero-1989)*  
Convocatoria: B.O.E. 8-Septiembre-1988. (Enero 1989 - Noviembre 1991).
- *Beca de Investigación de la Caja de Ahorros y Monte de Piedad de Madrid*  
3-Enero-1989. (Enero 1989 - Noviembre 1991).

- *Premio Extraordinario de Licenciatura de la Facultad de Ciencias Físicas*  
Curso 1987-88. Universidad de Valladolid, 19-Julio-1989.
- *Premio al Mejor Expediente Académico de la Facultad de Ciencias* convocado por la Caja de Ahorros y Monte de Piedad de Salamanca  
Curso 1987-88. Universidad de Valladolid, 31-Octubre-1989.
- *1<sup>er</sup> Premio Nacional de Terminación de Estudios de Ciencias Físicas*  
Curso 1987-88. B.O.E. 25-Octubre-1989.

**IV. ACTIVIDADES DE CARÁCTER CIENTÍFICO O PROFESIONAL**

- Oct. 85 - Oct. 88 *Colaborador Honorífico*  
Departamento de Física Teórica, Atómica, Molecular y Nuclear  
Facultad de Ciencias. Universidad de Valladolid.
- Ene. 89 - Oct. 91 *Becario de Investigación F.P.I.*  
Departamento de Física Teórica, Atómica, Molecular y Nuclear  
Facultad de Ciencias. Universidad de Valladolid.
- Oct. 91 - Dic. 93 *Profesor Titular Interino de Universidad*  
Área: Física Atómica, Molecular y Nuclear  
Departamento de Física Teórica, Atómica, Molecular y Nuclear  
Facultad de Ciencias. Universidad de Valladolid.  
Nº Registro de Personal : 0929448802 I0504
- Oct. 92 - Sep. 94 *Becario Postdoctoral MEC/FULBRIGHT y Research Associate*  
Department of Physics. University of California at Berkeley, y  
Materials Sciences Division, Lawrence Berkeley Laboratory.  
Berkeley, California, USA.
- Oct. 94 - Dic. 94 *National Science Foundation Fellow*  
Department of Physics. University of California at Berkeley, y  
Materials Sciences Division, Lawrence Berkeley Laboratory.  
Berkeley, California, USA.
- Apr. 98 - Sep. 98 *Profesor Visitante*  
Dpto. Física de Materiales  
Universidad del País Vasco, San Sebastian.
- 31.Dic.93-4-Abr.2001 *Profesor Titular de Universidad*  
Área: Física Atómica, Molecular y Nuclear  
Departamento de Física Teórica, Atómica, Molecular y Nuclear  
Facultad de Ciencias. Universidad de Valladolid.  
Nº Registro de Personal : 0929448802 A0504
- Nov. 00 - Feb. 01 *Profesor Visitante (Programa Sabático Salvador de Madariaga)*  
Laboratoire des Solides Irradiés, Ecole Polytechnique  
Palaiseau, Paris. Francia.
- Jun.05-Mar.06 *Profesor Visitante (Humboldt)*  
Freie Universität Berlin, Alemania
- Jun.07-Jul.07 *Profesor Visitante (1ere class des professeurs des unviersités)*  
Universidad de Montpellier 2, Francia
- 2009-2011 *Max-Planck Distinguished Visiting Scientist*  
i Fritz Haber Institute MPG  
Berlin, Alemania.
- Aug 14 - Sep. 14 *Miller Professor*  
Department of Physics. University of California at Berkeley  
Berkeley, California, USA.

## V. LÍNEAS DE INVESTIGACIÓN

The main activity of my research group is focussed on the field of theory and modelling of electronic and structural properties in condensed matter and on developing novel theoretical tools and computational codes to investigate the electronic response of solids and nanostructures to external electromagnetic fields. Present research activities are: new developments within many-body theory and TDDFT, including ab-initio description of electron excitations, optical spectroscopy, time-resolved spectroscopies, STM/STS, XAFS and lifetimes, novel techniques to calculate total energies and assessment and development of exchange-correlation functionals for TDDFT calculations; improvements on transport theory within the real-time TDDFT formalism; characterization of the electronic and optical properties of solids, nanostructures (in particular nanotubes, nanowires and semiconducting clusters) and biomolecules. The main research interest at present spans six main lines:

- Fundamental aspects of Time-Dependent Density Functional Theory and Many-Body Perturbation Theory
- Foundations of Time-dependent Density Functional Theory
- Foundations of Many-Body Theory
- Extended systems: solids, liquids, Applications (e. g. photovoltaics)
- Theory of Open quantum systems. Strong light-matter interactions and Optimal control Theory
- Theoretical Spectroscopy: photoemission, time-resolved optical and magnetic spectroscopies, Raman, IR ...
- Biotechnology and hybrid materials: photovoltaic applications
- Nanostructures and nanotubes. Nanocapilarity. Nanoplasmonics
- Electronic and Thermal transport
- Code development

The research is supported at present by different European Research Networks and projects and by the Spanish and Basque research agencies.

## VI. PARTICIPACIÓN EN PROYECTOS DE INVESTIGACIÓN SUBVENCIONADOS

1. *Estudio de la Estructura Electrónica y Atómica de Ciertos Materiales de Interés Tecnológico: Micropartículas Metálicas y Aleaciones Amorfas*  
(En colaboración con el Departamento de Física de la Materia Condensada, Universidad de Santiago de Compostela)  
DGICYT, Proyecto PB86-0654-C02 tres años (Octubre 1987-Octubre 1989). Dotación: 3.950.000 pts  
Investigador principal: J.A. Alonso
2. *Aleaciones y Micropartículas Metálicas: Estructura Electrónica de Pequeños Agregados Bimetálicos y Aleaciones Amorfas*  
DGICYT, Proyecto PB89-0352-C02-01 cuatro años (1990-1991-1992-1993). Dotación: 10.900.000 pts  
Investigador principal: J.A. Alonso
3. *Estructura Electrónica y Atómica del Enlace Químico en Algunos Materiales de Interés Tecnológico*  
Consejo Social de la Universidad de Valladolid, (1989). Dotación: 2.000.000 pts  
Investigador principal: J.A. Alonso.
4. *Propiedades Electrónicas, Magnéticas y Estructurales de Micropartículas Metálicas, Multicapas y Aleaciones Amorfas*  
Junta de Castilla y León tres años (1988-1989-1990). Dotación: 2.900.000 pts  
Investigador principal: L.C. Balbás.
5. *Propiedades Electrónicas, Magnéticas y Cohesivas de Ciertos Materiales de Interés Tecnológico: Pequeños Agregados Atómicos y Aleaciones Amorfas*  
Caja de Ahorros de Salamanca, (1989). Dotación: 500.000 pts  
Investigador principal: L.C. Balbás.
6. *Estudio Teóricos de la estructura Electrónica y Atómica de Ciertos Materiales de Interés Tecnológico: Micropartículas y Materiales Amorfos*  
Caja de Ahorros de Salamanca, (1990). Dotación: 500.000 pts  
Investigador principal: L.C. Balbás.
7. *Propiedades Electrónicas de Pequeños Agregados Atómicos Bimetálicos y de Multicapas*  
Proyecto de Cooperación Científica con Iberoamérica. Dotación: 500.000 pts  
Investigadores Principales: J.A. Alonso y J.L. Morán López (1990).
8. *Magnetismo en Capas Superpuestas de Metales de Transición*  
Acciones Integradas Hispano-Francesas HF-2B (área TM), tres años (1990-1991-1992).  
Ministerio de Educación y Ciencia.  
Subdirección General de Cooperación Internacional.  
Investigadores principales: L.C. Balbás y H. Dreyssé.
9. *Propiedades Electrónicas de Agregados Metálicos.*  
Ayuda a Investigación como Estímulo a Grupos Jóvenes de la Universidad de Valladolid, (1991).  
Dotación: 300.000 pts  
Investigador Principal: M.J. López.
10. *Theory of the Electronic Structure of Metal Clusters and Glasses*  
Financiado por la NATO (International Scientific Exchange Programs): Collaborative Research Grant, dos años (1990-1991). Dotación: 8000 USA \$  
Colaboración con Universität Osnabruck, Fachbereich Physik. Alemania.  
Invesigadores principales : G. Borstel y J.A. Alonso.
11. *Estudio de la estructura Electrónica y Propiedades Magnéticas de Superficies y Multicapas de Metales de Transición*  
Ministerio de Educación y Ciencia.  
Subdirección General de Cooperación Internacional.  
Cooperación con la Universidad de San Luis de Potosí (México).  
Instituto de Física Teórica (1992).  
Investigadores principales : J.L Morán-López y L.C. Balbás

12. *Compuestos Metálicos de Baja Dimensionalidad: Estructura Atómica y Electrónica e Implicaciones en Procesos de Magnetización y Catálisis Química*  
Junta de Castilla y León. Programa de Apoyo a Proyectos de Investigación (área de Nuevos Materiales), tres años (1991-1992-1993). Dotación: 1.800.000 pts  
Investigador Principal: L.C. Balbás
13. *Propiedades Electrónicas y Estructurales de Sistemas Metálicos.*  
Ayuda a Investigación como Estímulo a Grupos Jóvenes de la Universidad de Valladolid, (1992).  
Dotación: 300.000 pts  
Investigador Principal: **Angel Rubio**.
14. *Temperature Dependent Electronic Structure of Magnetic Solids*  
Acción Integrada Hispano-Alemana. dos años (1993-1994).  
Ministerio de Educación y Ciencia.  
Subdirección General de Cooperación Internacional.  
Investigador principal: W. Nolting
15. *Quantum Theory of Clusters and Solids*  
National Science Foundation (NSF) Grant No. DMR91-20269 y Director Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy (DOE) under Contract No. DE-AC03-76SF00098.  
Investigador Principal: M.L. Cohen
16. *Propiedades Estructurales, Electrónicas y Magnéticas de Materiales Metálicos: Agregados, Nanoestructuras y Sólidos*  
DGICYT, Proyecto PB92-0652-C03 tres años (Junio 1993-Junio 1996). Dotación: 13.000.000 pts  
Investigador principal: J.A. Alonso
17. *Propiedades Estructurales, Electrónicas y Magnéticas de Agregados Atómicos*  
Proyecto para Grupos Jóvenes de la Universidad de Valladolid, (1994). Dotación: 300.000 pts  
Investigador Principal: J.M. López.
18. *Excitaciones Ópticas de Agregados Metálicos y Semiconductores: Estudio Dentro del Funcional de la Densidad*  
CESCA (Centro de Supercomputación de Cataluña). (1995-2000) (1100 horas de computación).  
Investigador Principal: J.A. Alonso.
19. *Non-linear Effects in the Optical Properties of Atomic Clusters*  
Proyecto de la Dirección General de Investigación de Portugal. tres años (1996-1998).  
Grupos participantes: Coimbra, Valladolid, Milano, Roma, Buenos Aires  
Investigador Principal: J.M. Pacheco, coordinador en Valladolid: **Angel Rubio**
20. *Síntesis de Agregados Atómicos de Carbono, Nitrógeno y Boro, y Estudio de sus Propiedades Térmicas y Estructurales en Fase Gaseosa y Cristalina*  
Premio o Ayuda a la Investigación de la Fundación Domingo Martínez, (1996). Dotación: 2.000.000 pts  
Investigador Principal: J.A. Alonso.
21. *Simulation des Propriétés Structurales et Electroniques du Carbone ou de Composites en Nanotubes, en vue D'Applications Technologiques*  
CNUSC-Université de Montpellier, (3000 horas de computación). 1996-1997  
Investigador Principal: Patrick Bernier y **Angel Rubio**
22. *Estructura y Propiedades Ópticas de Nuevos Materiales de Interés Tecnológico: Heteroagregados Metálicos*  
Junta de Castilla y León. Programa de Apoyo a Proyectos de Investigación, (VA25/95) tres años (1995-1997).  
Dotación: 2.790.000 pts  
Investigador Principal: **Angel Rubio**
23. *Agregados Atómicos de Carbono, Nitrógeno y Boro: Estudio Teórico y Experimental de Una Nueva Familia de Materiales Avanzados en Ingeniería*  
Junta de Castilla y León. Programa de Apoyo a Proyectos de Investigación, (VA72/96) tres años (1996-1998).  
Dotación: 1.685.300 pts  
Investigador Principal: J.A. Alonso.



24. *Estudio Teórico de Nanoestructuras y Agregados Atómicos*  
DGES, Proyecto PB95-0720-C02-01 tres años (Sep. 1996-Sep. 1999). Dotación: 13.500.000 pts  
Investigador Principal: J.A. Alonso.
25. *Nuevos Métodos ab-initio para el Cálculo de Propiedades Físicas en Sistemas de Gran Tamaño. Aplicaciones Estratégicas en Semiconductores, Superficies y Macromoléculas Biológicas*  
DGES, Proyecto PB95-0202 tres años (Nov. 1996-Nov. 1999). Dotación: 10.600.000 pts  
Investigador Principal: J.M. Soler
26. *Cluster Formation in Liquid Alloys*  
NATO grant CRG.961128 un año (1997). Dotación: 280.000 F Belgas  
Investigadores Principales: J.A. Alonso y M. Stott (Queen's University, Kingston, Canadá).
27. *Estancia del Profesor M.J. Stott en Valladolid (Mayo-Junio 1997)*  
Programa Cátedra. Fundación BBV. Dotación: 700.000 pts  
Investigador Principal: J.A. Alonso
28. *Métodos de Espacio Real para las Excitaciones Electrónicas*  
Acción Integrada España-Reino Unido. dos años (Abril 1997-Abril 1999).  
Ministerio de Educación y Ciencia.  
Secretaría de Estado de Universidades e Investigación.  
Investigador Reino Unido: R. W. Godby (University of York)  
Investigador Español: Angel Rubio Dotación: 995.000 pts
29. *Simulación ab-initio de las Propiedades Estructurales y Electrónicas de Nuevos Materiales con Aplicaciones Tecnológicas: Nanotubos y Semiconductores*  
C<sup>4</sup> (Centre de Computació i Comunicacions de Catalunya). seis años (1997-2003) (120.000 horas de computación)  
Investigador Principal: Angel Rubio
30. *Simulation des Propriétés Structurales, Electroniques, Magnetiques, Mecaniques et Elastiques du Carbone ou de Composites en Nanotubes, en vue D'Applications Technologiques*  
IDRIS (CRAY C98/C94) y CNUSC-Montpellier, (24000 horas de computación). 1998-2003  
Investigador Principal: Patrick Bernier y Angel Rubio
31. *Nanotubes for Microstructure Technology (NAMITECH)*  
Training and Mobility Research Program of the EC TMR network contract ERBFMRX-CT96-0067 (DG12-MIHT) cuatro años (Julio,1996-Diciembre,2000). Dotación: 238.000 €  
Coordinador General: P. Bernier. Coordinador Español: Angel Rubio.
32. *Caracterización Teórica y Diseño de Nuevos Materiales con Propiedades "A Medida" para Aplicaciones Tecnológicas: Nanotubos y Nanoestructuras de Boro, Carbono y Nitrógeno*  
Junta de Castilla y León. Programa de Apoyo a Proyectos de Investigación, (VA28/99) tres años (1999-2001).  
Dotación: 3.165.000 pts  
Investigador Principal: Angel Rubio
33. *Nanotubos y otras Nanoestructuras con Interés Tecnológico*  
DGES, Proyecto PB98-0345 tres años (Dec. 1999-Dec. 2002). Dotación: 9.500.000 pts  
Investigador Principal: J.A. Alonso.
34. *Coupled Mechanical and Electronic Properties of Carbon Nanotubes based Systems (COMELCAN)*  
Research Training Network of the EC RTN network contract HPRN-CT-2000-00128 cuatro años (Marzo,2000-Febrero,2004). Dotación: 200.000 €  
Coordinador General: P. Bernier. Coordinador Español: Angel Rubio.
35. *Nanoscale Photon Absorption and Spectroscopy with Electrons (NANOPHASE)*  
Research Training Network of the EC RTN network contract HPRN-CT-2000-00167 cuatro años (Julio,2000-Junio,2004). Dotación: 192.000 €  
Coordinador General: R.W. Godby. Coordinador Español: Angel Rubio.

36. *Self-Assembly of Carbon Nanotube Junctions in Liquid Environments for Nanoelectronic Devices* (SATUNET)  
Research and Technological Development Projects of the EC RTD-FET network contract Number IST-2000-26361 un año (Septiembre,2000-Agosto,2001). Dotación: 20.000 €  
Coordinador General: D. Kern. Coordinador Español: **Angel Rubio**.
37. *Red Nacional de Investigaciones en Nanociencias: Metodologías Experimentales y Teóricas (NANOCIENCIA)*  
DGES, Proyecto PGC2000-2586-E tres años (Junio,2001-Abril,2004). Dotación: 5.000.000 pts  
Coordinador: Pedro Serena.
38. *Immobilization of Radionuclides in Oxides*  
MSCF Proposal (CPU time at EMSL), U. Washington (2001-2003). Investigador Principal: H Jonsson and **Angel Rubio**
39. *G4 DNA-Based Conducting Wires (G4DNA)*  
Information Society Technologies (IST) Program of the EC, contract Number IST-2000-29690 un año (2001).  
Dotación: 100.000 €  
Coordinator: D. Porath (Spanish coordinator **Angel Rubio**)
40. *Experimental and Theoretical Studies of Intercalated and Intracalated Carbon Nanotubes: An International Collaboration with EU-funded Researchers*  
Grant Number: NSF DMR-0100273, Department of Materials Science, University of Pennsylvania, Philadelphia, PA, 19104-6272, USA  
Principal Investigators: David E. Luzzi and Louis A. Girifalco
41. *Excitaciones Electrónicas en Nanoestructuras y Superficies*  
Grupos Consolidados y Alto Rendimiento, UPV/EHU cuatro años (2001-2005). Referencia: 9/UPV 00206.215-13639/2001 Dotación: 532.897 Euro  
Investigador Principal: P.M. Echenique.
42. *Teoría de Excitaciones Electrónicas en Nanoestructuras y Superficies (TEENS)*  
Programa Nacional de Materiales, Ministerio de Ciencia y Tecnología, Proyecto MAT2001-0946 tres años (2002-2004). Dotación: 31.300.000 pts  
Investigador Principal: P.M. Echenique.
43. *DNA-Based Molecular Nanowires (M-DNA)*  
Information Society Technologies (IST) Program of the EC, contract Number IST-2001-38051 tres años (2003-2005). Dotación: 18.000 €  
Coordinator: D. Porath (Spanish coordinator **Angel Rubio**)
44. *Nanomateriales para Aplicaciones Multisectoriales (NANOMAT)*  
ETORTEK-Proyectos de Investigación Estratégica sobre Nanotecnologías, Gobierno Vasco, tres años (2002-2004). Dotación (DIPC): 123.000 €  
Participants: LBEIN; DIPC; INASMET; POLYMAT.
45. *Towards the setting up of a Network of Excellence in Nanotechnology in Construction (NANOCONEX)*  
European Community Contract Number G1MAT-2002-04016. un año (2003). Dotación Total: 305.256 €
46. *Nanoscale Quantum Simulations for Nanostructures and Advanced Materials (NANOQUANTA)*  
Network of Excellence under the NMP3 priority of the European Commission's 6th Framework Programme.  
Contract Number NMP4-CT-2004-500198. cuatro años (Mayo 2004-2008) Dotación: 515.000 € Coordinador General: R.W. Godby. Coordinador Español: **Angel Rubio** and Pedro Echenique.
47. *Magnetic Interaction in BxCyNz Nanotubes and Derivatives*  
Project accepted in the Molecular Foundry, Berkeley (2004)  
Coordinators: C. Goze, and **Angel Rubio**
48. *Respuesta dinámica en nanoestructuras y sistemas de baja dimensionalidad*  
Programa Nacional de Promoción General del Conocimiento, Proyecto FIS2004-06490-C03 tres años (2005-2007). Dotación: 274620 Euros  
Investigador Principal: P.M. Echenique.

49. *Lattice Dynamics of Hexagonal Boron Nitride (h-BN) by Inelastic X-ray Scattering*  
European Synchrotron Radiation Facilities (ESRF); Beamline Round Beam time allocated ID28 (4/2005) 24 shifts, Proposal number: HS-2915 Co-proposers: J. Serrano, A. Bossak, R. Arenal, L. Wirtz, **Angel Rubio**
50. *Nanomateriales multifuncionales (NANOMATERIALES)*  
Convocatoria proyectos ETORTEK 2005: Ayudas a la investigación Estratégica (Dirección de Tecnología) tres años Enero 2005-Diciembre 2007.  
Investigador responsable: P. M. Echenique Dotación 233.588 € al DIPC.
51. *NANOTRON - Nanociencia y nanotecnología para micro y nanosistemas*  
Convocatoria proyectos ETORTEK 2005: Ayudas a la investigación Estratégica (Dirección de Tecnología). Proyecto: IE05-146 tres años Enero 2005-Diciembre 2007. Investigador responsable: P. M. Echenique Dotación 370.052 € Gobierno Vasco y 185.026 Diputación Foral de Gipuzkoa.
52. *Theoretical and computational study of ground state and excited state properties of nanostructured materials*  
Italian Ministry for Education, University and Research (MIUR), international project involving Rome, Paris, Milan, York, Berlin, San Sebastian. 80.000 Euros  
Investigador Principal in San Sebastian: **Angel Rubio**; Coordinador Italiano Prof. R. Del Sole
53. *Integrated Self-Adjusting Nano-Electronic Sensors (SANES)*  
Specific Targeted Research (STREP) under the NMP3 priority of the European Commission's 6th Framework Programme Information Society Technologies - 'IST' Contract number: NMP4-CT-2006-017310 tres años (April-2006-2009) Dotación: 172660 €  
Coordinador General: A. Kukovec. Coordinador Español: **Angel Rubio**
54. *CIC NanoGUNE Consolider* (Creación de un nuevo centro de I+D para la coordinación, desarrollo y gestión de las investigaciones en nanociencias del País Vasco  
Spanish Ministerio de Educación y Ciencia (Grant No. CSD2006-53) cinco años (15.09.2006 a 15.09.2011)  
Dotación: 4.500.000 €
55. *Probing Hierarchical Self-Assemblies Relevant for Drug and Vaccine Design by Employing STM*  
EU ERA-CHEMISTRY Project tres años (1/10/2006-30/09/2009) Dotación: 114.000 € Investigador Principal Español: **Angel Rubio** (en colaboración con B. A. Hermann (Munich) and P. H. Seeberger (Zurich))  
Acciones Complementarias: CTQ2005-25205-E y CTQ-2006-27171E
56. *COST ACTION MP0802 " Self-assembled guanosine structures for molecular electronic devices"*, Chair: Dr. Lea Spindler , Vice-chair: Dr. W. Fritzsche (2010-2012)
57. *DNA-based Nanoelectronics Devices (DNA-NANODEVICES)*  
STP Specific Targeted Research Projects of the Information Society Technologies - 'IST' (IST-2006-029192) (European Commission's 6th Framework Programme) (May 2006- 31-August-2010) Dotación: 55.000 €  
Coordinator: D. Porath (Spanish coordinator **Angel Rubio**)
58. *Aplicaciones en la frontera de la espectroscopia teórica: nanoestructuras y sistemas complejos (FANCYNANO)*  
Proyecto Coordinado del Ministerio de Educación y Ciencia (MEC) tres años (1/10/07-30/09/2010) (FIS2007-65702-C02-01) Dotación: 234.256 €  
Investigador Principal y Coordinador del Proyecto global: **Angel Rubio**
59. *Consolidación de la "European Theoretical Spectroscopy Facility (ETSF)" en España*  
Proyecto del Ministerio de Educación y Ciencia (MEC) (Acción Complementaria J) un año (1/12/07-30/11/08) (NAN2007-29370-E) Dotación: 30.000 €  
Investigador Principal: **Angel Rubio**
60. *Proyectos de la Red Española de Supercomputación*  
Investigador Principal: **Angel Rubio**  
QCM-2016-2-0017, QCM-2015-3-0017, QCM-2014-3-003: Analysis of the ultrafast charge transfer in organic photovoltaic devices based on endohedral metallofullerenes  
QCM-2015-1-0043: Modelling 2D Transition Metal Dichalcogenide Heterostructures  
FI-2015-1-0008: Real Space Real Time method for first principles calculations of general periodic systems using OCTOPUS  
QCM-2014-2-0036 Improving the Performance of the IO and Density Fragment procedures on OCTOPUS code.  
QCM-2014-1-0041 New local multipole implementation and visualization for Octopus code

QCM-2013-3-0007; QCM-2013-2-0045, QCM-2013-3-0007:: Performance of Time Dependent Density Functional Theory in the strong field photoionisation of noble gas atoms

QCM-2013-2-0042: Ultrafast Electron Dynamics at alkali/ice structures adsorbed on Cu(111) from experiments and theory

QCM-2013-2-0037, QCM-2013-3-0019: Ab-initio calculations of thermoelectric properties in nanostructures: silicene, germanene, Si/Ge heterostructure, and two-dimensional transition-metal-dichalcogenides

QCM-2013-1-0043: Quantum nonlocal effects in plasmonic nanostructures: bridging the gap between fully atomistic approaches and the classical descriptions of their electronic response

QCM-2013-1-0025: Ultrafast Electron Dynamics at alkali/ice structures adsorbed on Cu(111) from experiments and theory

FI-2013-1-0010: Octopus GS and TD scaling testing in new architectures

QCM-2012-3-0028: Quantum nonlocal effects in plasmonic nanostructures: bridging the gap between fully atomistic approaches and the classical descriptions of their electronic response

QCM-2012-3-0033: Ultrafast Electron Dynamics at alkali/ice structures adsorbed on Cu(111) from experiments and theory

QCM-2012-1-0034 Optical response, excitons and electronic correlations in TiO<sub>2</sub> nanomaterials: novel insights from a fully ab-initio many-body perturbation theory approach

QCM-2012-1-0029 Towards a novel oxide electronics: ab initio many body calculation of the electronic properties of interfaces between transition metal oxides

QCM-2011-3-0013: Optical, electronic and dynamical properties of confined water in carbon nanotubes

QCM-2011-3-0011: Towards a novel "oxide electronics": ab initio many body calculation of the electronic properties of interfaces between transition metal oxides

QCM-2011-3-0035: Defects mediated enhancement of TiO<sub>2</sub> photocatalysis in the visible range: understanding of the wet electron states by ab initio techniques

QCM-2011-3-0029: First principles study of the Supramolecular assembly of conductive 1D Pt-based structures

QCM-2011-3-0034: Optical response of silver nanoparticles to femto- and attosecond pulses: the role of the nanoparticle size and geometry"

QCM-2011-1-0039: Excited state properties of TiO<sub>2</sub> hybrid surfaces: photocatalysis and photovoltaics through ab initio many body Methods

QCM-2010-3-0012: Characterization of the optical absorption spectrum of Cationic porphyrins stacked in DNA derivatives by means of Time Dependent Density Functional Theory

FI-2010-3-0001: Towards understanding strong electronic correlation in transition-metal oxides from first principles: a theoretical spectroscopy approach

FI-2009-2-0026; FI-2009-3-0009; FI-2010-1-0002; FI-2010-2-0020: Optical and Charge Transfer Properties of Hybrid Organic-Dye/Oxide Nanostructure and Interface Systems for Solar Cells Application (ETSF activity)

FI-2009-1-0006; FI-2008-3-0014; FI-2008-2-0035: Optical Properties of BN Nanotubes and Hexagonal BN (ETSF activity)

FI-2007-3-0024; FI-2007-2-0012; FI-2007-1-0011; FI-2006-4-0017: Spectroscopic properties of biomolecules, nanostructures and extended systems (ETSF activity)

61. *Modeling photosynthesis from first principles*

Forschungszentrum Julich, Germany. Assigned 3 million core hours in the Jugene Petaflop Supercomputer for testing and code development, and access to the full machine once the code is prepared. Researchers: X. Andrade, M. A. L. Marques and A. Rubio. (2010-2011)

62. *Simulación de Nanoestructuras, Biomoléculas y sistemas complejos de interés tecnológico: técnicas espectroscópicas. ETSF en España*

Grupos Consolidados y Alto Rendimiento, UPV/EHU. Gobierno Vasco, Convocatoria de Ayudas para apoyar las actividades de los grupos de investigación del sistema universitario vasco (IT-319-07) seis años (2007-2012) Dotación: 601934.5€

Investigador Principal: **Angel Rubio**

63. *Etude des proprietes physiques des nanomateriaux a base de carbone*

Agencia Española de Cooperación Internacional AECI PCI-Mediterraneo (A/9817/07) (2008) Dotación: 4500 €

Investigador Principal: **Angel Rubio**

(en colaboración con Faculte des sciences (Muknes) Prof. Abdelali Rahmani)

64. *European Theoretical Spectroscopy Facility I3-ETSF*

Combination of Collaborative Project and Coordination and Support Action of the FP7 e-Infrastructure program

- (INFRA-2007-1.2.2 - Deployment of e-Infrastructures for scientific communities), Grant Agreement Number 211956 tres años (Enero 2008- June 2011) Dotación: 479.900 €  
 Coordinador General: R.W. Godby. Coordinador Español: **Angel Rubio**.
65. *Doping and temperature dependence of the Kohn anomaly in the phonon dispersion of graphite*  
 European Synchrotron Radiation Facilities (ESRF); Beamline Round Beam time allocated ID28 (1/2008) 24 shifts, Proposal number: HS-16169 Co-proposers: . A. Gruneis, T. Pichler, L. Wirtz and **Angel Rubio**
66. *Establecimiento de la Vicepresidencia científica de la ETSF en el País Vasco*  
 Acción Especial de investigación del Departamento de Universidades e Investigación del Gobierno Vasco, 2008-2009 (AE-2008-1-23) Dotación: 12000 €  
 Coordinador: **Angel Rubio**
67. *Desarrollo de la infraestructura científica de cálculo de la Vicepresidencia Científica de la European Theoretical Spectroscopy Facility (ETSF) en San Sebastián*  
 Acción Especial Cofinanciada del CSIC (MP/1926-mf), Centro Física de Materiales, Centro Mixto CSIC-UPV/EHU (2008-2009) Dotación: 50000 €  
 Coordinador: **Angel Rubio**
68. *Consolidación de la infraestructura científica de la ETSF en San Sebastián*  
 Proyecto Red Guipuzcoana de Ciencia y Tecnología e Innovación, Diputación Foral de Gipuzkoa (Ref: 47/08) (2009) Dotación: 30000 €  
 Coordinador: **Angel Rubio**
69. *Investigación estratégica en nanociencia y nanotecnología integrada en el centro de investigación cooperativa en nanociencias CIC nanoGUNE (inanoGUNE)*  
 Convocatoria proyectos ETORTEK 2008: Ayudas a la investigación Estratégica (Departamento de Industria, Comercio y Turismo de Gobierno Vasco). Proyecto IE08-225 tres años Enero 2008-Diciembre 2010.  
 Proyecto IE09-243 tres años Enero 2009-Diciembre 2011.  
 Investigador responsable: J.M Pitarke  
 Investigador responsable grupo UPV/EHU-ETSF **Angel Rubio** Dotación Grupo: 110469 €(Total: 3.149.498€).
70. *Understanding cohesive forces in nanosystems*  
 Australian Research Council Discovery Projects (ARC) (Grant DP1096240) tres años (2010-2012)  
 Coordinador Australiano: J. Dobson . Coordinador Español: **Angel Rubio**. Dotación 343000 \$ Australianos.
71. *Convenio Ikerbaske: ETSF*  
 Ikerbasque Foundation, cuatro años (2010-2013)  
 Coordinador: **Angel Rubio** Dotación: 145000 €.
72. *Thermal management with carbon nanotube architectures (THEMA)* RDG Small or medium-scale focused research project under the NMP priority of the European Commission's 7th Framework Programme FP7-NMP-2008-SMALL-2 Contract number: 228539 tres años (2010-2012) Dotación: 272.744 €  
 Coordinator: K. Kordas (Spanish coordinator **Angel Rubio**)
73. *Desarrollo de la Vicepresidencia Científica de la European Theoretical Spectroscopy Facility (ETSF)*  
 ACI promociona, MICINN (Diciembre-2009-Diciembre 2011) (ACI2009-1036) Dotación: 108.000 €  
 Investigador Principal: **Angel Rubio**
74. *Polymer based hybrid nanomaterials for photovoltaics: Improving efficiency by theoretical Modeling (POLYPHEMO)*  
 Funded by the Italian Institute of Technology (1-May-2010,30-April-2013) Dotación: 390.000 €  
 Co-ordinator in Italy: Dr. A. Mattoni  
 Co-director in Spain: **Angel Rubio**
75. *Estudio de la dinámica de sistemas cuánticos complejos: desde el desarrollos teóricos fundamentales a aplicaciones energéticas (captura, almacenamiento y transmisión)*  
 (Dynamical processes in complex quantum systems: from theoretical developments to energy harvesting and storage (DYNAPLEX))  
 Proyecto Coordinado del Ministerio de Ciencia e Innovación (MICINN) tres años (1/1/11-30/6/2014) (FIS2010-21282-C02-01) Dotación: 176.500 €  
 Investigador Principal y Coordinador del Proyecto global: **Angel Rubio**

76. *International collaboration in chemistry: molecules at nanostructured surfaces for solar cell applications*  
Programa Nacional de Internacionalización de la I+D Subprograma: proyectos internacionales (proyectos bilaterales EEUU) (PIB2010US-00652) tres años (1/12/2010-30/11/2012) Dotación: 210.500 €  
Investigador Principal Franz Himpfel, Enrique Ortega y A. Rubio
77. *Tailoring Electronic and Phononic Properties of Nanomaterials: Towards Improved Thermoelectricity (nanoTH-ERM)*  
Programa Consolider-Ingenio 2010, Ministerio de Ciencia e Innovación (Grant No. CSD2010-00044) cinco años (1.1.2011 a 31.12.2015) Dotación: 385.000 €(Total 3.900.000 €)  
Research coordinator: Clivia Sotomayor Torres
78. *Dynamical processes in open quantum systems: pushing the frontiers of theoretical spectroscopy (DYNamo)*  
European Research Council (ERC) Advanced Grant (ERC-2010-AdG -Proposal No. 267374) cinco años (1.4.2011 a 31.3.2016) Dotación: 1.877.497 €  
Investigador Principal: **Angel Rubio**
79. *Computer simulations of thermally excited molecules and materials by first principles (TEMM1P)*  
International Research Staff Exchange Scheme (FP7-PEOPLE-2011-IRSES)(grant 295172) cuatro años (2012-2015)  
Dotación: 29400 €  
Coordinator: Dr. T. Heine (Jakobs University, Germany)  
Co-ordinator in Spain: **Jesus Ugalde and Angel Rubio**
80. *CRONOS. Time dynamics and Control in nanostructures for magnetic recording and energy applications*  
FP7-NMP-2011-SMALL-5 "Modelling of ultrafast dynamics in materials" (Contract Number: 280879-2 CRONOS CP-FP7) tres años (June-2012-2015) Dotación: 232600 €  
Coordinator: Dr. S. Sanvito (Trinity College, Dublin)  
Co-ordinator in Spain: **Angel Rubio**
81. *POCAONTAS. Polymer / Carbon Nanotubes Active Systems*  
Marie Curie Actions Initial Training Networks, FP7-PEOPLE-2012-ITN (Project number 316633) cuatro años (1-Nov-2012-31-Oct-2016) Dotación: 237,296.62€  
Coordinator: Dr. L. Lauer (IMDEA, Madrid)  
Co-ordinator in San Sebastian: **Angel Rubio**
82. Marie Curie Actions-Intra-European Fellowships (IEF) ( FP7-PEOPLE-2011-IEF, Project: 302603) "Electron Correlation-Electron Correlation - The Electronic Ground State of Graphene Nanoribbons", Dr. Daniel Rohr (2013-2015) Host in Spain: **Angel Rubio** 168,896.40 €
83. Marie Curie Actions-International Incoming Fellowships (IIF) (FP7-PEOPLE-2012-IIF, Project: 326435) "First-principles theory of spatial dispersion in electromagnetic response of solids: Applications to natural optical activity and magnetoelectric effect (RespSpatDisp)", Dr. Irina V. Lebedeva (2013-2015) Host in Spain: **Angel Rubio** 166,336.20 €
84. *Plasmon dispersion in layered transition-metal dichalcogenides(TMDC)*  
European Synchrotron Radiation Facilities (ESRF); Beamline Round Beam time allocated ID20 (6/2013) 18 shifts, Proposal number: HC-730 Co-proposers: Simo Houtari, Pierluigi Cudazzo, Matteo Gatti and, **Angel Rubio**
85. *LHC-ABS - The optical absorption spectra of a real Light Harvesting Complex from first-principles: the spinach case*  
7th PRACE Call for project access, 21.560.000 core hours on MARENOSTRUM (BSC, Spain) (3-Sep-2013; 2-Sep-2014)  
Coordinator : **Angel Rubio**
86. *COST ACTION CM1204 "XUV/X-ray light and fast ions for ultrafast chemistry (XLIC)* Chair: Dr. M. Alcamí, Vice-Chair P. Bolognesi (2013-2016)
87. *Simulación de sistemas cuánticos nanoestructurados fuera del equilibrio: desarrollos fundamentales y aplicaciones energéticas (fotosíntesis artificial, materiales fotovoltaicos, interfaces orgánico-inorgánico, óxidos correlacionados, termoelectricidad, electrónica molecular)*  
Grupos Consolidados y Alto Rendimiento, UPV/EHU. Gobierno Vasco, Convocatoria de Ayudas para apoyar

- las actividades de los grupos de investigación del sistema universitario vasco (IT578-13) seis años (2013-2018)  
 Dotación: 538398€  
 Investigador Principal: **Angel Rubio**
88. *COST ACTION MP1306 "Modern tools for spectroscopy on advanced materials: a European modelling platform (EUSpec)"*  
 Chair: H. Ebber, Member of the Management Committee: **A. Rubio** (2014-2016)
89. *Desarrollos fundamentales para la simulación y caracterización de procesos dinámicos fuera del equilibrio en sistemas moleculares: materiales para aplicaciones energéticas (FUNEMAT)*  
 Proyecto Coordinado del Ministerio de Economía y Competitividad (MINECO)) tres años (1-1-2014;31-12-2016)  
 (FIS2013-46159-C3-1-P) Dotación: 129.470,00 €  
 Investigador Principal y Coordinador del Proyecto global: **Angel Rubio**
90. *2D Materials and Devices beyond Graphene Science & Emerging Technology of 2D Atomic Layered Materials and Devices, US Air Force*  
 The Air Force Office of Scientific Research (AFOSR): Awarded Grant No. FA2386-15-1-0006 AOARD 144088,  
 Funding 120000 \$ (Feb-2015-2017)  
 Principal Investigator in Spain **Angel Rubio**
91. *Marie Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2014, Proposal ID: 657424*  
 "QuantumLaP (Quantum Effects in Multicolor Ultrafast Laser Processing: Broadening Boundaries of Classical Descriptions)", Dr. Derrien Thibault(2015-2017)  
 Host in Germany (Hamburg): **Angel Rubio** 142721 €
92. *Marie Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2014, Proposal ID 660231*  
 "Electrical Spin Manipulation in Atoms and Molecules (SpinMan)", Dr. Andrea Droghetti(2015-2017) Host in  
 Spain: **Angel Rubio** 166,336.20 €
93. *Modelling stability of organic phosphorescent light-emitting diodes (MOSTOPHOS)*  
 H2020-NMP-2014: Widening Materials Models Proposal number: SEP-210187476 tres años (June-2015-2018)  
 Dotación: 242,689 €  
 Coordinator: Dr. D. Andrienko (Max Planck Institute for Polymer Research, Mainz )  
 Co-ordinator in Spain: **Angel Rubio**:
94. *Nanoscience foundries and fine analysis for Europe (NFFA-EUROPE)*  
 Call: H2020-INFRAIA-2014-2015 "Integrating and opening research infrastructures of European interest"  
 Project number: 654360, (2015-2019) Dotación: 127553 € Coordinator: Prof. Giorgio Rossi, Co-ordinator in  
 Spain: **Angel Rubio**
95. *The Novel Materials Discovery (NOMAD) Laboratory H2020-EINFRA-5-2015, Centers of Excellence for Computing applications ( Grant agreement number — 676580 — NoMaD) (1-11-2015-2018) Dotación: 1544,228€*  
 Coordinator: Prof. Matthias Scheffler Co-ordinator at MPSD (Hamburg): **Angel Rubio**
96. *Marie Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2015, Proposal ID 701796*  
 "Density Functional Theory for Thermoelectirc Phenomena (ThermalDFT)", Dr. Florian Eich (2016-2018)  
 Host in Hamburg (MPSD) Germany: **Angel Rubio** 159640,80 €
97. *Marie Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2015, Proposal ID 702406*  
 "Correlated Electron-Nuclear Dynamics: A novel mixed quantum-semiclassical approach (CoEND)", Dr. Ali Abedi (2016-2018)  
 Host in Spain: **Angel Rubio** 170121,60 €
98. *Marie Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2015, Proposal ID 702418*  
 "Strong Field Dynamics of Atoms and Molecules: History-dependent Functionals and Exact Kohn-Sham Potentials of the Time-dependent (multi-component) Density Functional Theory (AMO-dance)", Dr. Elham Khosravi (2016-2018) Host in Spain: **Angel Rubio** 170121,60 €
99. *Marie Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2015, Proposal ID 706890*  
 "Thermodynamics of Quantum Transport (QFluctTrans)", Dr. Cesar A. Rodriguez-Rosario (2016-2018)  
 Host in Spain: **Angel Rubio** 170121,60 €

100. *Marie Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2015, Proposal ID 706890*  
 ”Spin-Orbit Coupling at Interfaces from Spintronics to new Superconducting effects (SOCISS)”. Dr. Juan Borge de Prada (2016-2018)  
 Host in Spain: **Angel Rubio** 158121,60 €
101. *Marie Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2015, Proposal ID 746520*  
 ”Modelling 2D Transition Metal Dichalcogenide Heterostructures (MODHET)”, Dr. Lede Xian (2017-2019)  
 Host in Hamburg (MPSD) Germany: **Angel Rubio** 159640 €
102. *Quantum Spectroscopy: exploring new states of matter out of equilibrium (QSpec-NewMat)*  
 European Research Council (ERC) Advanced Grant (ERC-2015-AdG -Proposal No. 694097) cinco años  
 (1.10.2016 a 30.9.2021) Dotación: 2.492.500 €  
 Investigador Principal: **Angel Rubio**
103. *Nano Ionic Conducting Engineered materials for information application (NICE)*  
 Funded by: DFF-Research Project Grants from the Danish Council for Independent Research — Technology and Production Sciences Duration: 1/1/2017 to 31/12/2019 (3 years) Awarded Amount: DKK 5,801,760 (779.302 €) PIs: **J.M. Lastra and A.Rubio**
104. *Transporte Electrónico, Térmico, y de Espin con la Teoría de Funcionales de Densidad (SELECT-DFT)*  
 Proyectos EXCELENCIA del Ministerio de Economía y Competitividad (MINECO)) tres años (29-12-2016;31-12-2019) (FIS2016-79464-P) Dotación: 91.000,00 €  
 Investigador Principal: Stefan kurth and R. D’Agosta
105. *Marie Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2016, Proposal ID 751047*  
 ”Modelling superconductivity and spin-related effects in hybrid molecular/two-dimensional materials (Super-SpinHyMol)”, Dr. Jose Baldovi (2018-2019)  
 Host in Hamburg (MPSD) Germany: **Angel Rubio** 159460,80 €
106. *Marie Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2016, Proposal ID 753874*  
 ”Excitonic quasiparticles in Titania”, Dr. Adriel Dominguez (2017-2019)  
 Host in Spain (UPV/EHU) : **Angel Rubio** 158121,60 €
107. *Marie Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2016, Proposal ID 793609*  
 ”Topological New Fermions under Laser and New Topological Material Exploring via Machine Learning (TNFL-TMML)”, Dr. Peizhe Tang (May-2018-2020)  
 Host in Hamburg (MPSD) Germany: **Angel Rubio** 171460,80 €
108. *Marie Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2016, Proposal ID 795246*  
 ”Controlling Photoinduced Transitions with Strong Light Pulses in Condensed Matter (StrongLights)”, Dr. Joaquim Jornet-Somoza (Oct-2018-20)  
 Host in Hamburg (MPSD) Germany: **Angel Rubio** 171460,80 €
109. Shunsuke Sato Alexander von Humboldt Fellow – 01.05.2017-31.05.2019, 82800 €
110. Simone Latini Alexander von Humboldt Fellow – 01.06.2018 – 30.06.2020 82800 €
111. *QuantERA ERA-NET Cofund in Quantum Technologies*  
 RouTe 13N14839 (Jul-2018; Jun-2021) PI in Hamburg (MPSD) Germany: **Angel Rubio** 130634 €
112. *DFG Priority Programme SPP 1840: Quantum Dynamics in Tailored Intense Fields (QUTIF)*  
 ”SOLids in Strong Terahertz and Infrared CE-phase-stable waveforms” (SOLSTICE) (August-2018;July-2021)  
 Principal Investigator: **Franz Kaertner, Angel Rubio** 194650 €
113. *DFG Graduate School*  
 Research Training Group (RTG) -Quantum Mechanical Materials Modelling - QM<sup>3</sup> (Jan-2017;Dec-2019)  
 Principal Investigator in Hamburg: **Angel Rubio** 160000 €
114. *DFG Germany’s Federal Excellence Initiative*  
 Cluster of Excellence “Advanced Imaging of Matter” (AIM) (Jan.2019 – Dec.2025), Integrated Research Project B3.1 Principal Investigator: **Angel Rubio** 828 000€/per subproject



115. *Max Planck – New York City Center on “non-equilibrium Quantum Phenomena”* (2019-2023) Principal Investigator: **Angel Rubio** 4.828000 €
116. *DFG Collaborative Research Center SFB925*  
 “Light induced dynamics and control of correlated quantum systems”  
 (Jul 2019 – Jun 2023), Project A7 Principal Investigators: **Francesca Calegari, Angel Rubio** 101750 €
117. *Marie-Sklodowska-Curie Innovative Training Network SMART-X*  
 “Study of carrier transport in Materials by time-Resolved SpecTroscopy with ultrashort soft X-ray light”  
 (Jan2020 – Dec 2023) Principal Investigator: **Angel Rubio** 252788,40 €
118. *Fundamental Theoretical Materials Science (FunTheMaS)*  
 Grupos Consolidados y Alto Rendimiento, UPV/EHU. Gobierno Vasco, Convocatoria de Ayudas para apoyar las actividades de los grupos de investigación del sistema universitario vasco (IT1249-19) seis años (2018-2021)  
 Dotación: 325500€  
 Investigadores Principales: Stefan Kurth and **Angel Rubio**
119. *Marie Sklodowska-Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2019, Proposal ID 895747*  
 ”Novel molecular spectroscopies by nanoconfined light shaping and ab initio quantum dynamics (NanoLight-QD)”, Dr. Franco Bonafe (April-2020-22)  
 Host in Hamburg (MPSD) Germany: **Angel Rubio** 162806,40 €
120. Dongbin Shin, Alexander von Humboldt Fellow – 01.09.2020-31.08.2022 82800 €
121. *Marie Sklodowska-Curie Individual Fellowships (IF) Call: H2020-MSCA-IF-2019, Proposal ID 886291*  
 ” Photo-excited State Dynamics and Non-equilibrium States under Laser in Van der Waals Stacked Twodimensional Materials (PeSD-NeSL)”,”, Dr. Jin Zhang (April-2020-22)  
 Host in Hamburg (MPSD) Germany: **Angel Rubio** 174806,40 €

## VII. PUBLICACIONES O DOCUMENTO CIENTÍFICO-TÉCNICOS

**CLAVE:** L = libro completo, CL = capítulo de libro, A = artículo, R = review, E = editor, S = Documento Científico-Técnico restringido

## A. Artículos en Revistas de Investigación

1. L.C. Balbás, A. Rubio, J.A. Alonso y G. Borstel  
*Theoretical Study of the Stability of  $Ag_N^{2+}$ ,  $Ag_N^+$ ,  $Ag_N^-$  and  $Na_N$  Clusters as a Function of Size Using the Density-Functional Formalism*  
Chemical Physics **120**, 239-247 (1988) A
2. L.C. Balbás, A. Rubio, J.A. Alonso, N.H. March y G. Borstel  
*X-Ray Scattering Factors of Crystalline Silicon and Germanium from a Bond Charge Model*  
Journal of Physics and Chemistry of Solids **49**, 1013-1017 (1988) A
3. Ll. Serra, F. Garcias, M. Barranco, J. Navarro, L.C. Balbás, A. Rubio y A. Mañanes  
*The Static Polarizability of Metal Clusters and Spheres in a Improved Thomas-Fermi Approximation*  
Journal of Physics Condensed Matter **1**, 10391-10405 (1989) A
4. M.P. Iñiguez, J.A. Alonso, A. Rubio, M.J. López y L.C. Balbás  
*Dissociation Channels of  $Na_N^+$  Clusters ( $3 \leq N \leq 37$ )*  
Physical Review B **41**, 5595-5601 (1990) A
5. A. Rubio, L.C. Balbás y J.A. Alonso  
*Polarizabilities of Aluminum Clusters*  
Solid State Communications **75**, 139-142 (1990) A
6. Z. Penzar, W. Ekardt y A. Rubio  
*Temperature Effects on the Optical Absorption of Jellium Clusters*  
Physical Review B **42**, 5040-5045 (1990) A
7. A. Rubio, L.C. Balbás y J.A. Alonso  
*Density Functional Study of Neutral and Charged Sodium and Lead Clusters in the Jellium Model*  
Physica B **167**, 19-32 (1990) A
8. A. Rubio, L.C. Balbás, Ll. Serra y M. Barranco  
*Static Dipole Polarizability of Alkali-Metal Clusters: Electronic Exchange and Correlation Effects*  
Physical Review B **42**, 10950-10964 (1990) A
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6. *Theoretical Study of the Photoabsorption Spectrum of Na<sub>8</sub> and Cs<sub>8</sub>*  
21st Annual Symposium *Electronic Structure of Solids* and 75th WE-Heraeus-Seminar.  
Gaußig, Dresden, Alemania (11-15 Marzo 1991). 14-Marzo-1991
7. *Espectro de Fotoabsorción en Clusters Metálicos*  
II Reunión Nacional sobre Física de Micropartículas.  
Universidad de Valladolid (6-8 Mayo 1991). Valladolid. 6-Mayo-1991
8. *Método TB-LMTO para Clusters*  
II Reunión Nacional sobre Física de Micropartículas.  
Universidad de Valladolid (6-8 Mayo 1991). Valladolid. 7-Mayo-1991
9. *Aproximación No-Local a los Funcionales de Energía Cinética y de Intercambio*  
23 Reunión Bienal de la Real Sociedad Española de Física.  
Universidad de Valladolid (23-27 Septiembre de 1991). Valladolid. 23-Septiembre-1991
10. *Optical Properties of Metallic Clusters*  
Departamento de Física Moderna. Universidad de Cantabria. Santander. 16-October-1991
11. *Excitaciones Colectivas en Clusters*  
Departamento de Física Moderna. Universidad de Granada. Granada. 17-Marzo-1992
12. *Non-Local-Exchange-Correlation and Geometrical Effects in the Photoabsorption Cross Sections of Alkali Metal Clusters*  
Workshop on “*Dynamical Response of the Valence Gas in Simple Metal Systems*”.  
Villa Monastero, Varenna, Italia. 14-Mayo-1992
13. *Metallic Clusters: Electronic and Optical Properties*  
Department of Physics, University of California at Berkeley. California, USA. 4-Noviembre-1992
14. *Dipolar Response of Metallic Clusters*  
Department of Chemistry and Biochemistry, University of California at Los Angeles.  
Los Angeles, California, USA. 29-Enero-1993
15. *Weighted Density Approximation (WDA) for Electronic Calculations*  
Department of Chemistry, Durham. North Carolina, USA. 11-Mayo-1993
16. *Solid Made from Clusters*  
Department of Physics, University of California at Berkeley. California, USA. 27-Mayo-1993
17. *Response Properties of Metallic Clusters*  
Department of Physics and Tulane Quantum Group Seminar. New Orleans, Louisiana. USA. 30-Julio-1993
18. *Real Space Formalism for the Dielectric Matrix*  
Department of Physics, University of California at Berkeley. California, USA. 2-Junio-1994

19. *New Class of Nanotubes of Graphitic  $B_xC_yN_z$ : Electronic and Structural Properties*  
Xerox Palo Alto Research Center. Palo Alto. California, USA. 4-Noviembre-1994
20.  *$B_xC_yN_z$  nanotubes: Electronic and Structural Properties*  
Institut Romand de Reserche Numérique en Physique des Matériaux (IRRMA) IN-Ecublens.  
Lausanne, Suiza. 19-Abril-1995
21. *Predicción de Nuevos Materiales: Nanotubos de  $B_xC_yN_z$*   
E.T.S Ingenieros Industriales: “III Reunión de Materiales Avanzados: Nanotecnologías”.  
Valladolid 28-Abril-1995
22. *A Mixed-Space Formalism for Dielectric Response Calculations*  
Centre Europeen de Calcul Atomique et Moleculaire (CECAM).  
Lyon, Francia. 12-Julio-1995
23. *Mixed-space Formalism for the Dielectric Response in Extended Systems*  
Università degli Studi di Roma “Tor Vergata”, Dipartimento di Fisica.  
Roma, Italia. 29-Septiembre-1995
24. *Metal Intercalation in C and BN nanotubes*  
University of Coimbra, Department of Physics. Coimbra, Portugal. 22-Noviembre-1995
25. *Ab-initio Photoabsorption Spectra and Structures of Small Semiconductors and Metal Clusters*  
Schwäbisch Gmünd, Alemania. 20-Septiembre-1996
26. *Electronic and Doping Properties of  $B_xC_yN_z$  Nanotubes*  
NATO Advanced Research Workshop on *Nanowires*, Madrid, 24-Septiembre-1996
27. *Optical Response of Small Metallic and Semiconductor Clusters*  
*EXCAM Workshop*, Ecole Polytechnique, Paris. 26-Septiembre-1996
28. *Imaginary time calculations and Weighted-Density Approximation*  
*EXCAM Workshop*, Ecole Polytechnique, Paris. 27-Septiembre-1996
29. *Propiedades Electrónicas y Estructurales de Nanotubos*  
Instituto de Ciencias de Materiales-CSIC. Madrid. 13-Noviembre-1996
30. *Nanocomposite Tubules: Electronic and Structural properties*  
Ecole Polytechnique, Paris. 28-Noviembre-1996
31. *Response Functions in Extended and Low Dimensional Systems: Optical Absorption and Quasiparticles*  
Departamento de Física de Materiales, Facultad de Químicas, Universidad del Pais Vasco, San Sebastian. 12-  
Febrero-1997
32. *Nuevas Estructuras a Escala Nanométrica: Tubos de B-C-N*  
Departamento de Física, Universidad del Pais Vasco, Bilbao. 13-Febrero-1997
33. *Phenomenology of Metallic Resistivity in Carbon Nanotube Ropes*  
NAMITECH Workshop, Universidad de Valladolid. 19-Febrero-1997
34. *Properties of Composite Nanotubes and Selfinductance Effects in Chiral Tubes*  
NAMITECH Workshop, Universidad de Valladolid. 20-Febrero-1997
35. *Core Polarization in the Optical Response of Metal Clusters: Generalized Time-Dependent Density-Functional-Theory*  
Centre Europeen de Calcul Atomique et Moleculaire (CECAM).  
Lyon, Francia. 10-Septiembre-1997
36. *Electronic and Structural Properties of Nanotubes: Potential Applications*  
Groupe de Dynamique des Phases Condenses, Université de Montpellier II  
Montpellier, Francia. 6-Febrero-1998.
37. *(Mixed)-Space-Time Method for Response Calculations*  
Workshop: Dynamics of Clusters. Institute for Nuclear Theory, University of Washington  
Seattle, Washington (USA). 7-Julio-1998

38. *Self-inductance of chiral conducting nanotubes systems*  
Centre Europeen de Calcul Atomique et Moleculaire (CECAM).  
Lyon, Francia. 1-Septiembre-1998
39. *Electronic states in a finite carbon nanotube: a one-dimensional quantum box*  
Centre Europeen de Calcul Atomique et Moleculaire (CECAM).  
Lyon, Francia. 1-Septiembre-1998
40. *Nanotubes: A new class of materials*  
Física Estadística '99, Instituto de Física de Cantabria. 7-Mayo-1999
41. *Carbon Nanotubes: Electronic and Structural Properties*  
Fullerenes'99, Château Bonas, France. 31 Agosto 1999
42. *Spectroscopic Properties of Carbon Nanotubes*  
NanoteC99, University of Sussex, Brighton UK. 9 Septiembre 1999
43. *Optical Absorption and Inelastic Lifetimes in Noble Metals*  
MRS Fall Meeting Symposium: Computational Approaches to Predicting the Optical Properties of Materials.  
Boston, USA. 1 Diciembre 1999
44. *Nanotubos y Biofísica*  
IBGM, CSIC, Dpto. Bioquímica y Biología molecular. Facultad de Medicina. Universidad de Valladolid.  
4-Febrero-2000
45. *Theoretical Aspects of the Growth Mechanism*  
Workshop on "Nanotubes Growth Mechanisms: Experiments and Theory"  
Montpellier, Francia. 15-Mayo-2000
46. *Nanotubes: aplicaciones y propiedades*  
I Jornada sobre Nanotubos de Carbono.  
Dpto. Física Aplicada. Universidad de Alicante. 12-Junio-2000
47. *Nanotubes*  
Third Summer School of TMR network EMIT - "Light in, Sun out" - "Different aspects on the interaction of  
light with matter"  
Donostia International Physics Center, San Sebastian 28-Julio-2000
48. *Lifetimes of Hot Electrons in Metals*  
Psi-k 2000 Conference on "Ab Initio (from Electronic Structure) Calculations of Complex Processes in Materials"  
Schwäbisch Gmünd, Alemania. 24-Agosto-2000
49. *Electronic and (magneto)-transport properties of carbon nanotubes*  
Trends in Nanotechnology TNT2000, Toledo 17-October-2000
50. *TDDFT en sólidos y nanoestructuras: excitaciones ópticas*  
Departamento de Física Moderna. Universidad de Cantabria. Santander. 19-October-2000
51. *Nanotubos: nuevos materiales para aplicaciones en nanotecnología*  
Colloquium de la Facultad de Ciencias, Universidad de Santander. 20-October-2000
52. *Electron/hole Lifetimes in Metals*  
X International Workshop on Computational Material Science Total Energy and Force Methods  
Trieste, Italia 12-Enero-2001
53. *Electron/hole Lifetimes in Simple, Noble and Layered Metals*  
Laboratoire des Solides Irradiés, École Polytechnique, Palaiseau, Francia 16-Enero-2001
54. *Electronic and Structural Properties of Nanotubes*  
ONERA, Paris, Francia 20-Febrero-2001
55. *Nanotecnología: El futuro está en lo pequeño*  
Mesa Redonda sobre Nanotecnología. Palencia. 17,18-Julio-2001



56. *Structural Transformations in Carbon Nanotube Ropes*  
Trends in Nanotechnology TNT2001, Segovia 4-Septiembre-2001
57. *Electronic and Structural Properties of Nanotubes from First Principles*  
International Conference on the Applications of Density Functional Theory to Chemistry and Physics, El Escorial  
10-Septiembre-2001
58. *Time Dependent Density Functional Theory for the Optical Properties of Nanostructures and Solids*  
Particle-Solid Interactions. Euroconference on the Deposition of Atoms, Ions and Clusters at Surfaces, San  
Sebastián. 15-Septiembre-2001
59. *Nanotubos: Nuevos dispositivos a escala molecular*  
II Jornada científica del Instituto de Ciencia Molecular de la Universitat de Valencia, Valencia. 23-Noviembre-  
2001
60. *Young's modulus of carbon nanotubes: theoretical predictions*  
COMELCAN mid-term meeting and workshop on Mechanical Properties of Carbon Nanotubes. Max-Planck-  
Institut fuer Festkoerperforschung Sttugart, Alemania 17-19-Diciembre-2001
61. *Nanotubes: Electronic and Mechanical Properties*  
Max-Planck-Institut für Festkoerperforschung  
(Prof. K. Kern group seminar), Sttugart, Alemania 19-Diciembre-2001
62. *Propiedades electrónicas y estructurales de nanotubos*  
Universidad Autónoma de Madrid, 21-Febrero-2002
63. *Past/present/future of COMELCAN and related networks*  
European Community Young Researchers Meeting, Donostia, Spain. 6-Junio-2002
64. *Electronic and Structural Properties of BN tubes*  
NT02, Boston College, Boston, USA 6-Julio-2002
65. *Optical properties of nanostructures: a first-principles real-space-time approach*  
*Euroconference CMS02: XII Workshop on Computational Material Science*, Timi Ama, Sardinia, Italy 27-  
Septiembre-2002
66. *Optical properties of nanostructures and extended systems: a first-principle TDDFT approach*  
*Colloquium Institut für Theoretische Physik*  
Freie Universität, Berlin, Alemania 25-Noviembre-2002
67. *Structural, electronic and optical properties of C and BN nanotubes from first-principles*  
*Seminar of the Theory Department*  
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Alemania 26-Noviembre-2002
68. *Optical properties of biomolecules within TDDFT: excited state electron ion dynamics*  
"Theoretical Biophysics Symposium", Donostia, 5-7 March 2003 7-Marzo-2003
69. *Boron-Nitride Nanotubes*  
International Winterschool on Electronic Properties of Novel Materials Molecular Nanostructures  
(IWEPNM2003), March 8-15 (2003), Kirchberg/Tirol, Austria 13-Marzo-2003
70. *Spectroscopic Properties of C and BN Nanotubes: a First Principle Approach*  
MRS Symposium M: "Nanotube-Based Devices", San Francisco, California, USA, 21-25 Abril, 2003 22-Abril-  
2003
71. *Nanotubos: estructura, propiedades y aplicaciones en nanotecnología*  
Museo de la Ciencia, Madrid 24-Abril-2003
72. *Optical and Structural Properties of Nanotubes*  
Symposia : 'L - Carbon materials for active electronics' of the E-MRS 2003 Meeting,Strasbourg (France), June  
10-13, 2003 10-June-2003
73. *Optical response of nanostructures and bulk systems within Time-Dependent Density-Functional-Theory* Confer-  
ence on 'Ab-initio many-body theory for correlated electron systems' ICTP, Trieste (Italy) August 25-29 (2003).  
25-August-2003

74. *Optical, Infrared and STM spectroscopy of Carbon and BN nanotubes*  
TNT2003 "Trends in Nanotechnology" conference, Salamanca, (Spain) September 15-19 (2003) 17-Septiembre-2003
75. *Time dependent density functional approach to the calculation of the response properties of nanostructures*  
ADMOL, Advances in Molecular Electronics: From Molecular Materials to Single Molecule Devices, Dresden (Germany), February 23-27 (2004) 26-Febrero-2004
76. *Optical Properties of Boron-Nitride Nanotubes*  
International Winterschool on Electronic Properties of Novel Materials Molecular Nanostructures (IWEPNM2004), March 6-13 (2004), Kirchberg/Tirol, Austria 11-Marzo-2004
77. *Monitoring the Excited state electron-ion dynamics*  
Theoretical Challenges of 4th Generation Light Sources  
May 24-25, 2004, Abdus Salam International Centre for Theoretical Physics in Trieste, Italy 24-Mayo-2004
78. *Applications of TDDFT to the optical response of nanostructures and biomolecules*  
Electronic structure simulations of nanostructures (ESSN-2004): Towards and understanding of physical, chemical and biological processes  
June 18-21 2004, University of Jyväskylä, Finlandia 20-Junio-2004
79. *Nanotubos: presente y futuro en dispositivos nanométricos*  
Nanotecnologías en Electrónica, Encuentros Miramon, San Sebastián 28-Junio-2004
80. *TDDFT for optical absorption and electron energy-loss spectroscopy of nanostructures and extended systems*  
"Electronic Transport, Excitation and Correlation in Nano Science" from Oct 4-6, held at Hokkaido University in Sapporo, Japon. 5-October-2004
81. *Excitonic effects in the optical and energy-loss response of BN nanotubes*  
MRS Symposium II: "Modeling of one- and two-dimensional nanomaterials", Nov. 28, Dec. 3, Boston, USA. 30-Noviembre-2004
82. *Aplicaciones de la nanociencia: nanomotores moleculares y dispositivos*  
Curso Ciencia en Acción Nanotecnología, Enero-Marzo 2005, Koldo Mitxelena Kulturenea, San Sebastián 24-Febrero-2005
83. *¿ Para qué sirven los nanotubos?*  
Jornadas Convergencia Ciencia-Tecnología Alcalá de Henares 1-Marzo-2005
84. *Optical and ground state properties of solids within a GW-based OEP scheme*  
Workshop "Orbital Functionals for Exchange and Correlation", Berlin, House Christopherus 11-13 March 2005 13-Marzo-2005
85. *TDDFT for the response of nanostructures and solids*  
Centre for Computational Physics, Physics Department, University of Coimbra 6-Mayo-2005
86. *TDDFT-based formalism for the response of solids, nanostructures and biomolecules*  
EXCITING Symposium on Excited State Properties of Solids, Maritim Parkhotel Mannheim Germany May 16-19 (2005) 18-Mayo-2005
87. *Correlation effects in layered materials: an ACDFD first principle study (OEP)*  
CECAM workshop on "Van der Waals Forces and density functional theory", Lyon, France June 13-17 (2005) 15-Junio-2005
88. *TDDFT for the linear and non-linear response of nanostructures and solids*  
Colloquium of the Institute for Theoretical Physics, University of Regensburg, Germany. 7-Julio-2005
89. *Optical Properties of Nanostructures and Biomolecules from First Principles*  
Workshop on Metamaterials for Microwave and Optical Technologies, Palacio Miramar, San Sebastián. July 18-20 (2005). 20-Julio-2005
90. *A TDDFT-based formalism for the response of solids, nanostructures and biomolecules*  
356. WE-Heraeus-Seminar: "40 Years of the GW Approximation for the Electronic Self-Energy: Achievements and Challenges", Physikzentrum Bad Honnef, Bonn/Germany, 12-15 September (2005) 14-Sep-2005

91. *Optical properties of large organic molecules, nanostructures and biomolecules*  
Third Nanocose workshop (Nanocose 3), Villa Mondragone (Rome), October 3-5, 2005 4-October-2005
92. *First principle TDDFT description of the excited state properties bio-, nano- and extended systems*  
International Symposium on Surface Science and Nanotechnology, ISSS-4 Nov. 14-17, 2005, Omiya Sonic City, Japon 15-Nov-2005
93. *Response functions from a TDDFT-based formalism: applications to low dimensional structures*  
Colloquium of the MPI-PKS and the International Workshop on ATOMIC PHYSICS Nov.28-Dec. 2, 2005, Max-Planck-Institut für Physik Komplexer Systeme, Dresden 28-Noviembre-2005
94. *The world of nanotubes*  
*Physics-Colloquium*  
Freie Universität, Berlin, Alemania 9-Diciembre-2005
95. *A time-dependent density functional theory approach for the excited state dynamics of nanostructures and biomolecules*  
Symposium within the Division of Chemical Physics entitled Frontiers of Chemical Physics Theory  
March meeting of the American Physical Society, Baltimore USA 14-March-2006
96. *Excited state dynamics of nanostructures and biomolecules within TDDFT*  
Spring meeting of the DPG, Frankfurt, Alemania 17-Marzo-2006
97. *Weak interactions in layered materials within the ACDFE framework*  
van der Waals Workshop (vdW<sup>2</sup>) on Weak Chemical and Physical Interactions, 6-7 June 2006 SISSA, Trieste, Italy 7-June-2006
98. *Excited state dynamics of biomolecules from first principles*  
NANO2006 workshop on "Perspectives in Nanoscience and Nanotechnology" San Sebastian, Basque Country (Spain) on September 4-6, 2006 5-Septiembre-2006
99. *ICT and Physics: towards Atomic Scale technologies*  
Research Frontiers symposia, Information Science and Technology meeting IST2006 conference (Helsinki, November 21-23, 2006) 23 Noviembre 2006
100. *Boron nitride nanotubes*  
CAPE Advanced Technology Lectures and Seminars, Cambridge, UK 15-Diciembre-2006
101. *Spectroscopic Properties of hexagonal Boron Nitride and Nanotubes*  
International Winterschool on Electronic Properties of Novel Materials (IWEPNM2007), March 10-17 (2007), Kirchberg/Tirol, Austria 15-Marzo-2007
102. *Excited state properties of biomolecules*  
Progress in ab initio modelling of biomolecules : towards computational spectroscopy, Dipartimento di Fisica Università di Roma ( Roma, 2-4 April 2007), 3-April-2007
103. *BN nanotubes*  
CNR-INFN National Research Center S3 (nanoStructures and bioSystems at Surfaces) Modena, Italy 11-April-2007
104. *Theoretical description of the spectroscopic properties of biomolecules and nanostructures*  
Coloquio, Instituto de Ciencia Molecular (ICMol) Universidad de Valencia 24-Abril-2007
105. *Excited state properties of biomolecules: a TDDFT study* Coloquio del Institute for Biocomputation and Physics of Complex Systems, BIFI, Zaragoza, 11-Mayo-2007
106. *Applications of TDDFT to the response properties and excited state dynamics of solids, nanostructures and biomolecules*  
12th Density Functional Theory Conference, Amsterdam, The Netherlands, from 26-30 August 2007. 28-Agosto-2007
107. *Structural dynamics in the excite state within a tddft formalims*  
International Workshop on "Non-Adiabatic Dynamics at Surfaces" Schloss Reisenburg, Germany, 22-25. October 2007 24-October-2007

108. *Optical Properties of BN nanotubes and hexagonal BN: Role of Defects* Symposium II: Nanotubes and Related Nanostructures, 2007 MRS Fall meeting, 26-30 November 2007, Boston USA 28 November 2007
109. *Electronic properties of solids within a GW-based DFT scheme: Local versus non-local hybrid functionals* Symposium "Exact-exchange and hybrid functionals meet quasiparticle energy calculations" DPG spring meeting 2008, Berlin (25-29 February 2008) 28-Febrero-2008
110. *Dimensionality effects in the optics of BN nanostructures: role of defects* Nanospain 2008, Braga, Portugal 14-19 April 2008 16-Abril-2008
111. *Modelling the response to external stimulus of biomolecules* Biophysics Colloquium of the Center for Computational Physics Coimbra, Portugal 16-Abril-2008
112. *Electronic properties of nanostructures and biomolecules: excited state dynamics and molecular transport* A Thomas Young Centre Seminar at King's College London, London Centre for theory and simulation of materials 28-Mayo-2008
113. *Carbon nanotubes for renewable energy* Journée NAno EnR'08, Université Montpellier 2, France 4-June-2008
114. *Nanociencia: conceptos y aplicaciones* Garrigues Donostia 16-Junio-2008
115. *Optical Properties of BN nanostructures: role of Defects and dimensionality effects* NT08 (CCTN08 symposium) Montpellier Francia, 28 Junio-4 Julio (2008) 28-Junio-2008
116. *Understanding the properties of materials and nanostructures outside equilibrium: a time dependent density functional approach* 10th Granada Seminar on Computational and Statistical Physics: Modeling and Simulation of New Materials September 15-19, 2008 18-September-2008
117. *The world of nanotubes: new properties and applications* II workshop en Nanociencia y Nanotecnología Analíticas. Tarragona, 25-26 Septiembre 2008 25-Septiembre-2008
118. *State-of-the-art tools for state-of-the-art-users* "European Theoretical Spectroscopy Facility: The emergence of a new infrastructure", Louvain-la-Neuve, Belgium 28-Noviembre-2008
119. *Excited state dynamics of nanostructures and biomolecules within time-dependent DFT* Institute of Solid State and Materials IFW Dresden, Germany 22-January-2009
120. *What is the European Theoretical Spectroscopy Facility (ETSF) : the emergence of a new infrastructure* NFFA (Nanoscience Foundries and Fine Analysis) meeting, Centro Nacional de Microelectrónica (CSIC) Campus UAB, Spain 2-March-2009
121. *Boron Nitride and graphene nanostructures: properties and applications* NanoCenter Seminar, Pittsburgh, USA 17-March-2009
122. *Theoretical description of excited state dynamics in nanostructures* Symposium within the Division of Chemical Physics entitled "Structure and dynamics of interfacial water" March meeting of the American Physical Society, 16-20 March, Pittsburgh USA 18-March-2009
123. *Theoretical Spectroscopy of Complex Nanostructures and Biomolecules: Emergence of the ETSF* "Frontiers in Condensed Matter Physics and Nanoscale Materials" Symposium, in honor of Steven Louie's 60th birthday, 20-23 March Berkeley, USA 22-March-2009
124. *Understanding photophysical processes in biomolecules and nanostructures: recent developments and challenges* Colloquio of the Dipartimento di Fisica, Università "Tor Vergata", Rome, Italy 15-April-2009
125. *Theoretical spectroscopy of nanostructures and biomolecules* Colloquium of Institut für Physikalische Chemie Universität Würzburg, Germany 2-June-2009
126. *Boron Nitride nanotubes: properties and applications* E-MRS Symposium N "Carbon nanotubes and graphene low dimensional carbon structures", Strasbourg (France), June 8 to 12, 2009 10-June-2009

127. *Theoretical Spectroscopy of Complex Nanostructures and Biomolecules*  
XXIV International Conference on Photochemistry ICP2009, 19-24 July 2009 Toledo Spain 22-July-2009
128. *GW renormalization of DFT molecular electronic levels at the vicinity of a surface: The image charge effect*  
13th Intern. Conf. on the Applic. of Density Functional Theory in Chemistry and Physics, DFT09, 30-Aug to 4-Sep. Lyon, France. 31-Agosto-2009
129. *Excited state properties of BN nanotubes optical and energy loss spectroscopies*  
Workshop on Inorganic Nanotubes Experiment and Theory  
DIPC, San Sebastián, Septiembre 2-4, 2009 2-Septiembre-2009
130. *BCAM Seminar Efficient Implementation of time-dependent density-functional theory for the dynamical description of biomolecules and nanostructure*  
Basque Center for Applied Mathematics (BCAM), Zamudio, Spain 18-Septiembre-2009
131. *Boron Nitride and Carbon nanotubes*  
International Conference on Carbon Nanostructured Materials  
Santorini, Greece 4 - 8 October 2009 6-October-2009
132. *Challenges and Perspectives from (TD) Density Functional Theory: From Low-Dimensional Structures to Real Material*  
From Basic Concepts to Real Materials, 2-6 November 2009, UC Santa Barbara, Kavli Institute for Theoretical Physics 2-Noviembre-2009
133. *Efficient implementation of time-dependent density functional theory for biomolecules and nanostructures*  
Department of Mathematics, UC Santa Barbara, 9-Noviembre-2009
134. *Theoretical spectroscopy of low dimensional systems*  
Center for Excitonics, Cambridge, MIT, Harvard 11-Noviembre-2009
135. *Spectroscopy of complex nanostructures and biomolecules*  
SISSA & DEMOCRITOS National Simulation Center, Trieste, Italy 8-Abril-2010
136. *The European Theoretical Spectroscopy Facility and the spectroscopy of complex nanostructures and biomolecules*  
The International Workshop on Molecular Materials, Sanxenxo, Spain from 2nd to 5th May 2010. 3-Mayo-2010
137. *Theoretical Spectroscopy*  
Atomistic and Molecular Simulations, Challenges for the next decade  
Launching of the ZCAM "Zaragoza Scientific Center for Advanced Modeling", May 27-28 (2010) 28-May-2010
138. *Simulation the excite state dynamics of complex nanostructures and biocomplexes*  
Colloquium of the Max-Planck-Institut fuer Festkoerperforschung, Stuttgart 15-June-2010
139. *Tools for the users: ETSF (European Theoretical Spectroscopy)*  
Open e-IRG Workshop (organised under the Spanish Presidency of the European Union), Madrid, 17-June-2010  
17-June-2010
140. *Nanostructured materials: New charge transfer solids and optoelectronic devices*  
Abschieds-Kolloquium, FU Berlin, Fachbereich Physik, Berlin 1-July-2010
141. *Excited state dynamics of low-dimensional systems and biomolecules*  
FHI, Department of Physical Chemistry, Berlin 5-July-2010
142. *Efficient Formalism for Large Scale Ab Initio Molecular Dynamics and mixed quantum classical dynamics with the correct equilibrium distribution*  
 $\Psi_k$  Conference 2010, 12-16 September 2010, Berlin 14-September-2010
143. *First principle modeling of the excite state properties of complex nanostructures and biomolecules: a TDDFT and Many-Body perturbation theory approach*  
Passion for Knowledge, San Sebastian (27th-September 1st October 2010) 29-Septiembre 2010
144. *Microscopic modeling and design of nanostructured-based devices: from photovoltaics to light-emission*  
3rd European School on Molecular Nanoscience (ESMOLNA2010), Miraflores de la Sierra, Madrid, 24-29th October 27-October-2010

145. *Time-dependent DFT*  
HoW exciting! Hands-on workshop on excitations in solids employing the EXC!TiNG code, CECAM Lausanne, Switzerland, 11-17 November 15-November-2010
146. *Ab-initio modeling of nanostructured-based devices: from photovoltaics to nanotube light-emission*  
Colloquium of the Max-Planck-Institut fuer Mikrostrukturphysik, Halle 22-November-2010
147. *Ab-initio modeling of nanostructured-based devices for optoelectronic applications*  
Colloquium Fakultät für Physik, Universität Wien, Austria 14-March-2011
148. *Simulation of photo-induced processes in complex systems from first principles: role of electron correlations and dynamical screening*  
Colloquium at Center for Atomic-scale Materials Design (CAMD), Denmark 23-March-2011
149. *Modeling Photo-induced dynamical processes in massive parallel architectures*  
ImagineNano, HPC 2011 (High Performance Computing), BEC (Bilbao Exhibition Centre), Spain 11-14th of April 2011 14-April-2011
150. *Photo-induced dynamical processes in nanostructures, biomolecules and oxides*  
Colloquium CNR-NANO National Research Center S3 (nanoStructures and bioSystems at Surfaces) Modena, Italy, 27-April 2011
151. *Modeling photo-induced dynamical processes in complex nanostructures and oxides: role of electron correlations, dynamical screening and electron-phonon coupling*  
Elementary Processes in Solids and at Interfaces: Carrier, Lattice, and Molecular Dynamics (ElePSI), Kloster Banz, Germany 29-May, 1st June 2011 30-May-2011
152. *Properties and applications of inorganic nanotubes: the case of B-C-N*  
2011 TMCN, Transition Metal Chalco/Halide Nanostructure meeting, Lausanne, Switzerland June 6-8, 2011 7-June-2011
153. *Open problems with excitations in TDDFT*  
How to Speed Up Progress and Reduce Empiricism in Density Functional Theory June 20-24, 2011, ACAM, Dublin, Ireland 21-June-2011
154. *First principles simulation of the spectroscopic properties of low-dimensional systems*  
60th celebration of Hajo Freund and Matthias Scheffler "FIESTAE", 28-June, 1st-July (2011) 30-June-2011
155. *Modeling the electronic properties of nanotubes and biomolecules: towards nanostructured-based optoelectronic devices*  
Satellite Meeting "Theoretical Modelling of Materials" of 9th World Congress of the World Association of Theoretical and Computational Chemists (WATOC), Barcelona, 13-15 July 2011 15-July-2011
156. *Boron Nitride and graphene nanostructures: properties and optoelectronic applications*  
Columbia University (Depts of Physics and Electrical Engineering) 15-August-2011
157. *Light induced electron-hole photo-physical processes in nanostructures: open questions for TDDFT*  
Gordon Research Conference on "Time-Dependent Density-Functional Theory" August 14-19, 2011, University of New England, Biddeford, ME, USA 18-August-2011
158. *Light induced electron-hole photo-physical processes in nanostructures*  
Quantum Simulations and Design, International Focus Workshop- September 27 - 29, 2011, Max-Planck-Institut für Physik komplexer Systems, Dresden 27-September-2011
159. *Theoretical spectroscopy: modelling photo-induced dynamical processes in nanostructures and oxides*  
Theorie-Kolloquium wird von der Fachgruppe Theoretische Physik, Martin-Luther Universität Halle-Wittenberg, Germany 12-October-2011
160. *Theoretical concepts for the simulation of nanostructured-based devices: from photovoltaics to light-emission*  
4th European School on Molecular Nanoscience (ESMOLNA2011), Peñíscola, Spain 23-28th October 24-October-2011
161. *Modeling Nanostructured materials*  
Coloquium Institute of Solid State and Materials IFW Dresden, Germany, 10th November 2011

162. *Non equilibrium dynamical simulations of complex systems from TDDFT*  
Third Theory Days: Stochastic and Dissipative Effects , Toulouse, France, Nov-Dec 30, 2 1-December-2011
163. *Modeling optoelectronic nanostructured devices made of inorganic nanotubes*  
Colloquium Physics Department of the University Duisburg-Essen, Germany 14-December-2011
164. *Ultrafast response of solids and nanostructures investigated via many-body theory and time-dependent density functional techniques*  
Gordon Research Conference "Ultrafast Phenomena in Cooperative Systems, Understanding Complex Matter Far from Equilibrium and on Elementary Time Scales" February 19-24, 2012 Hotel Galvez Galveston, TX (USA) 22-February-2012
165. *TDDFT for nonlinear phenomena of light-matter interactions*  
Symposium within the Division of Chemical Physics entitled "Density Functional Theory for Chemical Physics" March meeting of the American Physical Society, February 27-March 2, 2012, Boston, MA, USA 1-March-2012
166. *Photodynamics of nanostructures: a TDDFT approach to the weak and strong coupling regimes*  
Colloquium of the Materials Physics Department , University of Oxford, England 10th-May-2012
167. *TDDFT for light-matter interactions in strong coupling regimes*  
2nd TYC workshop on energy materials, 6-8 June 2012, London, UK 7-June-2012
168. *Simulating optoelectronic devices at the nanoscale: a TDDFT perspective*  
2n International Conference on Advanced Materials Modelling (ICAMM), Institut des Matériaux Jean Rouxel, June 13-16, Nantes France 14-June-2012
169. *Unraveling the electronic properties of nanostructures and biomolecules from spectroscopy: a theoretical perspective*  
Concepts and Applications of Stimulus-responsive Materials  
Summer UPV/EHU Workshop, Donstia June 20-22 (2012) 21-June-2012
170. *Modeling photo-induced dynamical processes in nanostructures and biomolecules from first principles: correlation effects and applications*  
Colloquium of Center for Free-Electron Laser Science (CFEL), Hamburg, Germany 6th July 2012
171. *Perspectives*  
HoW exciting! Hands-on Workshop on Excitations 2012. HU Berlin, August 2-8, 2012 8-August-2012
172. *Hybrid organic photovoltaics: from a time-dependent density functional perspective*  
CECAM Conference: "Energy from the Sun: Computational Chemists and Physicists Take up the Challenge", 10-14 September, 2012, Chia Laguna resort, Cagliari, Sardinia Italy 14-September-2012
173. *Unraveling the electronic properties of nanostructures and biomolecules from spectroscopy*  
Mini workshop on "Electronic structure and optical properties of materials" to the memory of Prof. Rodolfo del Sole, Università di Roma Tor Vergata, Roma 15-September-2012
174. *Theoretical concepts for the simulation of nanostructured-based devices:towards nanostructured-based optoelectronic devices*  
NANOWIRES12, Paul-Drude-Institut, 19-21 September 2012 20-September-2012
175. *What time-dependent density functional theory can provide to understand and design nanostructured-based optoelectronics materials*  
Colloquium Department of Chemistry, Technische Universität München, Garching 18-October-2012
176. *Electronic properties of New Hybrids Made of BN and C*  
5th European School on Molecular Nanoscience (ESMOLNA2012), Cuenca, Spain 28th October-2nd November 2012 1st-November-2012
177. *Predicting properties of nanostructures and biomolecules*  
Public Lecture, University of Luxembourg, 12th-November-2012
178. *Understanding and designing of energy materials from first principles simulations: optoelectronic and hybrid-photovoltaic devices*  
Colloquium of the Physics Department, University of Luxembourg, 12th-November-2012

179. *Modelización en la Nanoescala*  
Simposio Fronteras de la Ciencia en Brasil y España, 10-12 Diciembre 2012, Universidad de Salamanca y Fundação de Amparo à Pesquisa do Estado de Sao Paulo 12 December 2012
180. *Fundamentals of TDDFT for nonlinear phenomena of light-matter interactions: application to hybrid organic photovoltaics and charge transfer processes*  
CECAM workshop "Calculation of Optical Properties of Nanostructures from First Principles", February 19-22, CECAM-HQ-EPFL, Lausanne, Switzerland 20-February-2013
181. *TDDFT for Nonlinear Light-Matter Interactions: Application to Hybrid Organic Photovoltaics and Charge Transfer Processes*  
Seminar of the Theory Department of the Fritz-Haber-Institut, Berlin 28-February-2013
182. *New nanoscale hybrid structures made of C and BN from first principles: optoelectronic devices*  
International Winterschool on Electronic Properties of Novel Materials (IWEPNM2013), March 2-9 (2013), Kirchberg/Tirol, Austria 3-March-2013
183. *How non linear and charge transfer processes are captured in time-dependent density functional theory*  
TD-DFT (Time-Dependent Density Functional Theory ) conference, University of Nantes, France, 23-26 April (2013) 23-April-2013
184. *Non equilibrium dynamical processes in finite and extended systems: a TDDFT and many-body perspective*  
Workshop on "Dynamics of Matter: Advances in Theory", CFEL, Hamburg 25-April-2013
185. *Time-dependent density functional theory for non-linear phenomena in solids and nanostructures: fundamentals and applications*  
Electronic structure calculations with the GPAW code: Users and developers meeting, Technical University of Denmark, May 21-23, 2013 22-May-2013
186. *A TDDFT perspective on nonlinear electronic processes: optics, photoemission and resonant tunneling*  
Workshop: "Learning from the past, looking to the future" from July 2-5, 2013 in Berlin, Germany 4-July-2013
187. *Static and time-dependent density-functional schemes for bond-breaking and bond formation, correlation effects including Mott insulators*  
Humboldt Universitaet zu Berlin, Institut fuer Chemie (AG Quantenchemie, Prof. Sauer) 10-July-2013
188. *Light-induced dynamical processes in finite and extended systems from TDDFT*  
Modeling Single-Molecule Junctions: Novel Spectroscopies and Control Berlin, Germany, October 14th - 16th, 2013 15-October-2013
189. *Non equilibrium dynamical processes in finite and extended systems from a time-dependent density functional (TDDFT) perspective*  
Max-Planck-Institut für Quantenoptik (MPQ) Colloquium, Munich 17-October-2013
190. *Impacto de la teoría en Nanociencia: nuevos materiales y dispositivos*  
Nanotecnología, Fundación Valenciana de Estudios Avanzados, Valencia 15-November-2013
191. *Non linear processes in low dimensional systems within time-dependent density functional theory*  
The "March" meeting, a symposium in honor of Professor Norman H. March. Namur, Belgium 21-23rd November 2013 22nd-November-2013
192. *Open session about challenges and standing problems*  
6th Time-Dependent Density-Functional Theory: Prospects and Applications, Benasque, 4-18 January 2014 13-January-2014
193. *Light-induced processes in finite and extended systems from TDDFT*  
VI International Conference of the Institute for Biocomputation and Physics of Complex Systems (BIFI), "Exploring the role of computation in Science: from Biology to physis", Zaragoza (Spain), January, 22-24, 2014. 22-January-2014
194. *Non equilibrium dynamical processes in low dimensional systems from a time-dependent density functional perspective*  
Colloquium of the Institut für Physikalische Chemie Universität Würzburg, Germany 11-February-2014



195. *Multi-scale modeling in chemistry and materials science: combining classical and quantum mechanics*  
Colloquium of the Instituto de Ciencia de Materiales de Madrid (ICMM), Madrid 20-February-2014
196. *Extensions of density functional theory approaches to treating quantum phenomena and quantum entanglement*  
March meeting of the American Physical Society (APS), March 3-7, 2014; Denver, Colorado, USA 3-March-2014
197. *Modeling energy materials from first principles simulations: optoelectronic and hybrid-photovoltaic devices*  
Colloquium of the Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain 28-March-2014
198. *Understanding light-induced processes in energy materials from first principles TDDFT simulations*  
Workshop on Material Challenges in Devices for Fuel Solar Production and Employment, ICTP, Trieste, Italy, 19-23 May (2014) 23-May-2014
199. *Modeling optoelectronic and hybrid-photovoltaic devices within TDDFT*  
Colloquium Physikalische Chemie, Department of Chemistry, Universität München 4th-June-2014
200. *Hybrid-organic photovoltaic devices from first principles simulations*  
White nights of materials science: From physics and chemistry to data analysis, and back, Saint Petersburg, Russia – June 16 - 20, 2014 hfill18-June-2014
201. *Non equilibrium light-induced dynamical processes in energy materials from first principles*  
2nd Workshop on Surfaces, Interfaces and Functionalization Processes in Organic Compounds and Applications - SINFO II Trieste, 25-27 June 2014 27-June-2014
202. *Optoelectronic and hybrid-photovoltaic devices from first principles simulations*  
Seminar of the Physical Chemistry department (ISIC) at the EPFL, Lausanne 12-July-2014
203. *Ab initio modelling of light-induced non equilibrium dynamical processes in organic materials*  
Department of Physics, Stanford University, USA 22-August-2014
204. *Efficient implementation of time-dependent density-functional theory to treat non-linear dynamical processes in molecular nanostructures and solids*  
Applied Mathematics Seminar, Department of Mathematics, University of California, Berkeley 3-September-2014
205. *First principles modeling of photovoltaic and optoelectronic devices: fundamentals and applications*  
Department of Chemistry, University of California, Berkeley, USA 12-September-2014
206. *Modeling non equilibrium dynamical processes in TDDFT: optoelectronic and photovoltaic applications*  
Physical Seminar, University of Rochester, USA 15-September-2014
207. *Non equilibrium dynamical processes in TDDFT: organic photovoltaic applications*  
Colloquium Molecular Foundry, Lawrence Berkeley Laboratory, Berkeley 16-September-2014
208. *Theoretical Spectroscopy: TDDFT*  
7th European School on Molecular Nanoscience (ESMOLNA2012), Gandia (Spain), 26th to 30th October 2014 27th-October-2014
209. *Novel electronic and structural properties of two-dimensional materials: silicene, germanene and stanene*  
"Emerging Non-Graphene 2D Atomic Layers and van der Waals Solids" Symposium of the Fall Materials Research Society (MRS) meeting, Boston, (November 30 - December 5, 2014). 3-December-2014
210. *Ab initio simulation of photon-matter interactions: non equilibrium dynamical processes within QED-TDDFT*  
Colloquium of Center for Free-Electron Laser Science (CFEL), Hamburg, Germany 7th November 2014
211. *TDDFT or how to describe non-linear dynamical processes in many-electron systems: quantum phenomena and quantum entanglement*  
Mini-Symposium "Formal and practical aspects of Electronic Structure Simulations with DFT", Department of Theoretical Chemistry Vrije Universiteit Amsterdam, The Netherlands 29-January-2015
212. *Simulation of photon-matter interactions within QED-TDDFT*  
SWOCS V, Symposium of Computational Science, POSCO International Center, Pohang, Korea 3-February-2015

213. *Non equilibrium dynamical processes in TDDFT: optoelectronic and photovoltaic applications*  
IBS Center for Multidimensional Carbon Materials , Ulsan National Institute of Science and Technology (UNIST), South Korea 4-February-2015
214. *Novel electronic and structural properties of two-dimensional materials: from carbon-nanostructures to silicene, germanene and stanene*  
IBS Center for Multidimensional Carbon Materials , Ulsan National Institute of Science and Technology (UNIST), South Korea 5-February-2015
215. *A TDDFT framework for describing light-induced non equilibrium dynamical processes: optoelectronic applications*  
Division of Materials Physics, Department of Physics University of Helsinki, Finland 25-March-2015
216. *Simulating strong light-matter interactions: a TDDFT perspective*  
Columbia University (Depts of Physics and Electrical Engineering) 30-April-2015
217. *Simulation of Optoelectronic and Photovoltaic processes within a TDDFT formalism*  
Colloquium of the Physical Chemistry department at EPFL, Lausanne 21-May-2015
218. *Modeling photon matter interactions within QED-TDDFT: optoelectronic applications*  
Colloquium University of Konstanz, Konstanz 2-June-2015
219. *Light induced non-linear dynamical processes in molecules and solids within TDDFT*  
The Batsheva de Rothschild Seminar on Molecular Electronics 2015: 40 Years Later, Orchid Jerusalem View Hotel (Maale Hachamisha), Israel 7-12 June 2015 8-June-2015
220. *Ab-initio simulations of light-matter interactions*  
XFEL Theory seminar, Hamburg 9-July-2015
221. *Pressure induced phase transition in correlated oxides and simple metals: Mott and charge-transfer insulators*  
Keynote Speaker AIRAPT-EHPRG "International Conference on High Pressure Science and Technology" Madrid 30-August-4-September 2015 3-September-2015
222. *Quantum Electrodynamical time-dependent density functional theory (QEDFT): an ab-initio framework for the simulation of photon-matter interactions*  
"3rd International Conference on Correlation Effects in Radiation Fields 2015" (CERF15) Sep. 13-18 in Rostock, Germany 18-September-2015
223. *Simulating light-induced dynamical processes in light harvesting complexes*  
"Chemistry, Materials & Light", in the framework of the International Year of Light IYL2015, Consiglio Nazionale delle Ricerche (CNR), Bologna, Italy, 21-23 September 2015. 22-September-2015
224. *Extending time-dependent density functional theory to account for many body photon-electron quantum phenomena: towards QED-chemistry*  
Exploration of ultra-fast timescales using time dependent density functional theory and quantum optimal control theory, September 28-October 2, 2015, CECAM-HQ-EPFL, Lausanne, Switzerland 30-September-2015
225. *Simulating light-induced dynamical processes within TDDFT: application to light harvesting complexes*  
3a jornada de supercomputación, Cátedra UAM-Fujitsu en Computación Científica y Big Data, Madrid, 23-October-2015
226. *First principle simulations of energy materials for optoelectronic and hybrid-photovoltaic applications*  
Colloquium of the Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain 15-October-2015
227. *Group IV two-dimensional materials : Novel electronic and structural properties*  
Colloquium Institute of Solid State and Materials IFW Dresden, Germany, 24th November 2015
228. *Extensions of time density functional theory to treat strong light-matter interactions and quantum entanglement*  
CECAM-SMEE Workshop on Open quantum Systems, November 30th - December 4th, 2015, The University of Hong Kong, China 2-December-2015
229. *A TDDFT formulation for strong light matter interactions : applications to energy conversion*  
Colloquium Institut fuer Theoretische Physik, Technische Universitaet Dresden, Dresden, Germany, 26-January-2016

230. *First principles modeling of light-induced ultrafast phenomena in nanostructures and solids*  
Workshop "The Frontier of ultrafast science: integrating XFEL and fs-TEM for a novel approach to time-resolved science" 1-3 February 2015, Trieste, Italy 2-February-2016
231. *Strong light-matter interactions and quantum entanglement: merging QED and TDDFT*  
Colloquium Nano/Bio Interface Center & Pennergy, University of Pennsylvania, Philadelphia, USA 16-February-2016
232. *Extensions of time density functional theory to QED: QED-Chemistry*  
DCP Symposium for the March 2016 Meeting of the APS in Baltimore. APS March Meeting 2016, March 14-18, 2016, Baltimore, MD. 15-March-2016
233. *Group IV two-dimensional materials : Novel electronic and structural properties*  
National Institute for Materials Science (NIMS) Colloquium, Tsukuba, Japan 4-April-2016
234. *Electronic and structural properties of 2D elemental materials: applications in nanoscience*  
Department of Physics, Tohoku University, Sendai, Japan, 7-April-2016
235. *Strong light-matter interaction and quantum entanglement: merging QED and TDDFT*  
National Institute of Advanced Industrial Science & Technology (AIST) Specialized Seminar, Tsukuba, Japan 11-April-2016
236. *Strong light-matter interaction in materials science: merging QED and TDDFT*  
Colloquium, Department of Physics Tokyo Institute of Technology, Oh-okayama Tokyo, Japan 12-April-2016
237. *Strong light-matter interaction in materials science: merging QED and TDDFT*  
Colloquium Institute for Solid State Physics, University of Tokyo Kashiwa, Tokyo, Japan 13-April-2016
238. *Strong light-matter interaction in materials science: merging QED and TDDFT*  
Colloquium Wako RIKEN, Japan 14-April-2016
239. *Strong light-matter interaction in materials science: merging QED and TDDFT*  
Colloquium Center for Computational Sciences University of Tsukuba, Tsukuba, Japan 15-April-2016
240. *Time-resolved angle resolved photoelectron spectroscopy within TDDFT: what can we learn and what are the limitations?*  
Focus Workshop: "Prospects and Limitations of Electronic Structure Imaging by Angle Resolved Photoemission Spectroscopy", 25-27 April 2016, Max Planck Institute for the Physics of Complex Systems MPIPES Dresden 26 April 2016
241. *Group IV two-dimensional materials : Novel electronic and structural properties* Physical Chemistry Colloquium, Caltech, USA 17-May-2016
242. *A Quantum of Light for Materials Science: merging QED and TDDFT* Materials Research Lecture, Caltech, USA 18-May-2016
243. *"New states of matter": merging quantum electrodynamics and TDDFT to model light-matter interactions*  
Special Seminar, Physic Departmnet, McCullough , Stanford university 23-August-206
244. *Modeling Light-Matter interaction: From Weak to Strong Coupling in QED Chemistry and Materials*  
Symposium on Frontiers in Physical Sciences, International Center for Advanced Studies (ICAS), 16-18 November 2016, Buenos Aires, Argentina 18-November-2016
245. *Modeling Light-Matter interactions: Quantum Electrodynamics (QED) Chemistry and Materials within TDDFT*  
18th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods, January 12-14, 2017, ICTP, Miramare, Trieste, Italy 12-January-2017
246. *Modeling Weak to Strong Coupling in QED Chemistry and Materials*  
Colloquium Institut für Theoretische Physik und Astrophysik Christian-Albrechts-Universität Kiel, Germnay 24-January-2017
247. *"New states of matter": merging quantum electrodynamics and TDDFT to model light-matter interactions*  
Colloquium at the Physics Department, Lund University, Sweden 28-February-2017

248. *Elemental two-dimensional materials : Novel electronic and structural properties*  
International Winterschool on Electronic Properties of Novel Materials Molecular Nanostructures (IWEPNM2017), March 4-11 (2017), Kirchberg/Tirol, Austria 9-Marzo-2017
249. *Ab-initio spin and time-resolved ARPES in real materials with QED-TDDFT: driving WSe2 out of equilibrium*  
Workshop on Spectroscopy and Dynamics of Photoinduced Electronic Excitations, ICTP, Trieste 8-12 May 2017  
11-May-2017
250. *First principles modeling of Light-Matter interactions within QED-TDDFT: From Weak to Strong Coupling in QED-Chemistry and Materials*  
Max-Planck-Institut für Quantenoptik (MPQ) Colloquium, Garching 6-June-2017
251. *QED-Chemistry and Materials: A First principles modeling of Light-Matter interactions within QED-TDDFT*  
29th Annual Workshop on Recent Developments in Electronic Structure Methods (ES17) June 25-28, 2017,  
Princeton University, USA 27-June-2017
252. *Floquet Topological Solids*  
University of Pennsylvania, Philadelphia, USA. 6-July-2017
253. *QED-Chemistry and Materials: A new theoretical framework for the first principles modelling of Light-Matter interactions, from weak to strong coupling*  
Colloquium Department of Chemistry and Chemical Biology, University of Harvard, Cambridge USA 10-July-2017
254. *First principles modeling of time-resolved ARPES in real materials with QED-TDDFT: driving WSe2 out of equilibrium*  
Condensed Matter and Biophysics Experimental Physics, MIT Cambridge USA 11-July-2017
255. *Non equilibrium driven phenomena in 2d materials from first principles*  
Workshop on Quasi-particle Dynamics in Quantum Confined and Emerging Materials Columbia University  
MRSEC, New York 14-July-2017
256. *Modeling out of equilibrium time-resolved ARPES in real materials with QED-TDDFT: application to WSe2*  
Department of Chemistry, Yale University 2-August-2017
257. *QED-Chemistry and Materials: First principles modeling of Light-matter interactions within QED-TDDFT*  
Mini-symposium on light-matter interactions, University of Strasbourg, 15-September-2017
258. *How photons change the properties of matter from an ab initio QED-TDDFT formalism*  
Zurich Theoretical Physics Colloquium, ETH Zurich, Switzerland 27-November-2017
259. *How photons change the properties of matter: QED-TDDFT an ab initio framework for modeling Light-Matter interactions*  
Plenary Talk at the Annual DPG Spring Meeting in Berlin, Germany, March 11th – 16th, 2018 (held jointly with the annual European Physical Society (EPS) Meeting of the Condensed Matter Divisions) 16th-March-2018
260. *Photons and matter cooperate: new states of matter from an ab-initio QED-TDDFT formalism*  
Strong Coupling with Organic Molecules (SCOM 2018), Eindhoven, April 16-18 (2018) 17th-April-2018
261. *Non equilibrium light driven phenomena in materials from first principles: merging quantum electrodynamics QED and TDDFT*  
Q-MAC Symposium, May 22 - 25, 2018, Venice, 23-May-2018
262. *QED-TDDFT: A new theoretical framework for the first principles modelling of Light-Matter interactions, from weak to strong coupling*  
Quantum electrodynamic effects/processes in molecules and materials "QED-M2", Collège de France, Paris,  
June 18-19 2018 18-June-2018
263. *Modeling light-induced ultrafast phenomena in nanostructures and solids*  
Symposium on 'Recent progress in Chemistry and in Advanced Materials', at the David Lopatie Conference  
Centre, Weizmann Institute of Science (Israel) 28th-October-2018

264. *How photons change the properties of matter: QEDFT a first principles framework for modeling light-matter interactions*  
 "Quantum and Classical Light-Matter Interactions" CUNY Graduate Center, New York 12-13 November 2018  
 12-November-2018
265. *Photons and matter cooperate: new states of matter from a novel first principles QEDFT formalism*  
 Zemansky Lecture at CUNY 14th November 2018
266. *New states of matter from an ab-initio QED-TDDFT formalism*  
 Colloquium of the Centre for Doctoral Training in Cross-Disciplinary Approaches to Non-Equilibrium Systems (CANES), London 19th-November-2018
267. *Quantum Electrodynamical Density Functional Theory (QEDFT): a novel theoretical framework for the simulation of photon-matter interactions*  
 "Ultrafast Science from the infrared to the X-rays", Rolex Centre of the Ecole Polytechnique Fédérale de Lausanne (EPFL), 28-30 November 2018 29-November-2018
268. *Photons and matter cooperate: new states of matter from QED-TDDFT*  
 Wednesday-Colloquium, Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, Frankfurt 16-January-2019
269. *New states of matter from a novel first principles quantum electrodynamics density functional formalism (QEDFT)*  
 Zernike Colloquium, Zernike Institute for Advanced Materials Colloquia, University of Groningen 17th February 2019
270. *Materials in QED cavities*  
 Q-MAC Symposium, 24 - 27, 2019, Paris, 'Fondation Hugot Du Collège De France 25-Feb-2018
271. *Quantum Electrodynamical Density Functional Theory (QEDFT): towards new states of matter*  
 Symposium in Honor of the 70th Birthday of Steven G. Louie, Berkeley USA 2-March-2019
272. *Modelling Floquet and Quantum-Cavity Engineered new states of matter*  
 Quantum Matter Physics Seminar, University of Geneva, Switzerland. 19th-March-2019
273. *Light and cavity induced new states of matter: Quantum Electrodynamical Density Functional Theory (QEDFT)*  
 Plenary Talk at the Annual DPG Spring Meeting in Rostock, Germany, March 10th – 15th, 2019 12th-March-2019
274. *Strong light-matter interaction and New States of Matter*  
 Centro Singular de Investigación en Química Biológica y Materiales Moleculares (CIQUS), Universidad de Santiago de Compostela 30th-April-2019
275. *Novel Electronic and Structural Properties of Two-Dimensional Materials and Floquet and cavity-engineering of molecular and materials properties*  
 Seminar in Harvard.School of Engineering and Applied Sciences.SEAS, Harvard, Cambridge, MA 27-28th June 2019
276. *Engineering materials properties with light*  
 Workshop "A light touch for quantum material control", Department of Physics, University of Oxford, UK , 5th July 2019 5-July-2019
277. *Cavity and Floquet-Engineered new states of matter*  
 Flatiron Seminar Series, New York 2-August-2019
278. *Quantum-Cavity and Floquet-Engineered new states of matter from a QEDFT perspective*  
 Molecular and materials simulation at the turn of the decade: Celebrating 50 years of CECAM (CECAM50). 9-12 September Lausanne, Switzerland 10-September-2019
279. *Floquet and cavity-engineered materials*  
 Department Seminar, Molecular Spectroscopy Group of the Max Planck Institute for Polymer Research Mainz, Germany 24-September-2019

280. *Cavity-engineering of molecular and materials properties from first principles QEDFT*  
Quantum light for investigating complex molecules and materials, Theo Murphy international scientific meeting,  
The Royal Society at Chicheley Hall, Buckinghamshire, 25-26 November 2019 26-November-2019
281. *Quantum cavities and Floquet materials engineering from first principles QEDFT*  
March meeting of the American Physical Society (APS), March 2-7, 2020; Denver, Colorado, USA 3-March-2020
282. *Floquet and cavity materials engineering: an ab initio QEDFT perspective*  
2020 International Conference on Low Energy Electrodynamics in Solids (LEES2020), The Westin in Portland,  
Maine June 28- July 3 29 June 2020
283. *Engineering materials properties with light: Floquet and cavity-engineered materials*  
CECAM-Workshop on "Real-time quantum dynamics in photo-stimulated processes: experiment and theory",  
Beijing Computational Science Research Center (CSRC), Beijing, China October 12-17,2020 14 October 2020
284. *"Cavity twistronics" a platform for quantum matter on demand*  
Physics Colloquium at Columbia University, NY 9-November-2020
285. *Engineering quantum materials with optical cavities and light: a QEDFT approach*  
CAMD Webinar , DTU Physics, Technical University of Denmark, Kgs Lyngby, Denmark 1-December-2020
286. *Cavity QED quantum materials engineering: "Cavity twistronics"*  
L4G Seminar at ICFO - The Institute of Photonic Sciences, Barcelona 11-December-2020
287. *Engineering quantum materials with optical cavities and light: "Cavity twistronics"*  
2nd Berkeley Excited States Conference (BESC2021) on January 7-8, 2021 7-January-2021
288. *Cavity control of two-dimensional materials phenomena*  
Polariton Chemistry Webinar , UC San Diego 17-February-2021
289. *Quantum materials engineering with optical cavities and light*  
Colloquium at the Imperial College Network on the Frontiers of Ultrafast Science, London 24-March-2021

## IX. CONTRIBUCIONES A CONGRESOS Y CURSOS CIENTÍFICOS

1. *21 Reunión Bienal de la Real Sociedad Española de Física*  
Salamanca, Octubre de 1987  
COMUNICACIONES / POSTERS (2).  
- *Estudio Teórico de la Estabilidad de los Clusters  $Ag_N^{2+}$ ,  $Ag_N^+$ ,  $Ag_N^-$  y  $Na_N$  como Función del Tamaño Usando el Formalismo del Funcional de la Densidad.* L.C. Balbás, A. Rubio, J.A. Alonso y G. Borstel  
- *Factores de Estructura de Silicio y Germanio Cristalinos.* A. Rubio, L.C. Balbás, J.A. Alonso, G. Borstel y N.H. March
2. *Fourth International Symposium on Small Particles and Inorganic Clusters*  
Aix en Provence, Francia, Julio de 1988  
COMUNICACIÓN / POSTER.  
- *Theoretical Study of the Stability of  $X_N^n$  ( $n=-1,0,+1,+2$ ;  $X=Ag,Cu$ ;  $N\leq 25$ ) Clusters as a Function of Size Using a Non-Local Density-Functional Formalism.* A. Rubio, L.C. Balbás y A. Vega
3. *El Universo a Cortas y Largas Distancias: Gran Unificación y Supercuerdas*  
Universidad Internacional Menéndez Pelayo (UIMP). Santander, 10-14 Agosto de 1987.  
ASISTENCIA.
4. *International Conference on Applications of Density Functional Theory to Chemical and Physical Properties of Inorganic Systems*  
Arles, Francia, Septiembre de 1988  
COMUNICACIÓN / CONFERENCIA INVITADA.  
- *Self-Consistent Weighted-Density-Approximation to Exchange-Correlation Potential in Atoms and Metallic Clusters.* L.C. Balbás y A. Rubio
5. *Charles Coulson Summer School in Theoretical Chemistry*  
Oxford University. Oxford, Inglaterra, 4-14 Septiembre de 1988.  
ASISTENCIA.
6. *Fourth International Workshop on Computational Condensed Matter Physics: "Total Energy and Force Methods"*  
International Centre for Theoretical Physics. Trieste, Italia, 4-6 Enero 1989.  
ASISTENCIA.
7. *Applications of Statistical and Field Theory Methods to Condensed Matter*  
NATO Advanced Study Institute. Evora, Portugal, 22-Mayo al 2-Junio de 1989.  
ASISTENCIA.
8. *Applications of Statistical and Field Theory Methods to Condensed Matter*  
NATO Advanced Study Institute. Evora, Portugal, 22-Mayo al 2-Junio de 1989.  
ASISTENCIA.
9. *Fusión Nuclear por Confinamiento Magnético*  
Universidad Internacional Menéndez Pelayo (UIMP). Santander, 28-Agosto al 2-Septiembre de 1989.  
ASISTENCIA.
10. *III Escuela Ibérica de Física de Materia Condensada. Magnetismo y Materiales Magnéticos*  
Jaca, 11-23 Septiembre de 1989.  
ASISTENCIA.
11. *XXII Reunión Bienal de Química*, Septiembre 1988.  
POSTER.  
- *La Termodinámica de los Gases Reales.* J. Casanova, A. Rubio, C.F. Nicolás y C. Casanova Roque
12. *22 Reunión Bienal de la Real Sociedad Española de Física*  
Palma de Mallorca. 1-7 Octubre de 1989.  
COMUNICACIONES / POSTERS (5).  
- *Estudio Teórico de la Afinidad Electrónica de Clusters de Aluminio.* A. Rubio, L.C. Balbás y J.A. Alonso  
- *Polarizabilidad Estática de Clusters de Sodio. Efectos de Intercambio y Correlación Electrónicos.* A. Rubio, L.C. Balbás, Ll. Serra y M. Barranco

- *Propiedades Magnéticas y Estructurales de Óxidos de Metales de Transición*. A. Vega, A. Rubio, J. Dorantes-Dávila y L.C. Balbás
  - *Propiedades Magnéticas de Heteroclusters de Metales de Transición*. A. Vega, A. Rubio, J. Dorantes-Dávila y L.C. Balbás
  - *Oscilaciones de Superficie en Agregados Metálicos*. Ll. Serra, F. Garcias, M. Barranco, J. Navarro, L.C. Balbás, A. Rubio y A. Mañanes
13. *Workshop: "Micropartículas Metálicas: Del Átomo al Sólido"*  
Universidad de Valladolid, 12-14 Febrero de 1990.  
CONFERENCIA INVITADA.
  14. *10th General Conference of the Condensed Matter Division of the European Physical Society*  
Lisboa, Portugal, 9-12 Abril de 1990.  
COMUNICACIÓN / POSTER.  
- *Temperature Effects on the Optical Absorption of Jellium Clusters*. Z. Penzar, W. Ekardt y A. Rubio
  15. *Interactions of Charged Particles with Solids and Surfaces*  
NATO Advanced Study Institute. Alicante, 6-18 Mayo de 1990.  
COMUNICACIÓN / POSTER.  
- *Influence of Thermal and Quantum-Mechanical Lattice Vibrations on the Measured-Plasmon Line-Widths in Small Simple Metal Clusters*. Z. Penzar, W. Ekardt y A. Rubio
  16. *II-Workshop on Magnetic Confinement Fusion: Transport and Confinement in Toroidal Devices*  
Universidad Internacional Menéndez Pelayo (UIMP). Santander, 2-6 Julio 1990.  
ASISTENCIA.
  17. *5th International Symposium on Small Particles and Inorganic Clusters (ISSPIC-5)*  
University of Konstanz, Konstanz, Alemania, 10-14 Septiembre de 1990.  
COMUNICACIONES / POSTERS (3).  
- *The Response of Metal Clusters to q- and L- Dependent External Fields*. Ll. Serra, F. Garcias, N. Barberán, M. Barranco, J. Navarro y A. Rubio  
- *The Static Polarizability of Metal Clusters*. Ll. Serra, F. Garcias, M. Barranco, J. Navarro, L.C. Balbás, A. Rubio y A. Mañanes  
- *Response Properties of Alkaline Clusters within a Jellium-like Model with Finite Surface Thickness*. A. Rubio, L.C. Balbás y J.A. Alonso
  18. *11th European Conference on Surface Science (ECOSS-11)*  
Universidad de Salamanca, Salamanca, 1-4 Octubre de 1990.  
COMUNICACIÓN / POSTER.  
- *Magnetic Properties and Stability of Multilayers and Semi-Infinite Systems of Cr(Fe) on Fe(Cr) (001) Surface*. J. Dorantes-Dávila, A. Mokrani, A. Vega, A. Rubio, H. Dreyssé y L.C. Balbás
  19. *Colloque "Couches Minces Magnetiques"*.  
Pont-à-Mousson, Francia, 20-22 Septiembre de 1990.  
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- *Détermination Autocoherente du Magnétisme de Surface et d'Interface par le Méthode de Réursion*. A. Mokrani, S. Bouarab, A. Vega, A. Rubio, L.C. Balbás, J. Dorantes-Dávila, C. Demangeat y H. Dreyssé
  20. *5th Symposium on Surface Physics*.  
Chlum Castle CS, Checoslovaquia, 8-12 Octubre de 1990.  
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- *Self-Consistent Determination of Surface and Interface Magnetism with the Recursion Method*. A. Mokrani, H. Dreyssé, J. Dorantes-Dávila, A. Rubio, A. Vega, L.C. Balbás y C. Demangeat
  21. *MMM-Conference*.  
San Diego, Estados Unidos, Noviembre de 1990.  
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- *Antiferromagnetic Interlayer Coupling in Fe/V and Fe/Cr*. A. Vega, A. Rubio, L.C. Balbás, J. Dorantes-Dávila, C. Demangeat, A. Mokrani y H. Dreyssé



22. *MRS Spring Meeting*.  
Anaheim, Estados Unidos, 29-Abril al 1-Mayo de 1991.  
COMUNICACIÓN ORAL.  
- *Magnetism of Stepped Surface and Interface*. J. Dorantes-Dávila, A. Vega, A. Rubio, L.C. Balbás, A. Mokrani, C. Demangeat y H. Dreyssé
23. *Workshop on Magnetic Materials and their Applications*.  
La Habana, Cuba, 21-30 Mayo de 1991.  
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- *Interface Magnetism in Fe/V and V/Fe Stepped Surfaces*. H. Dreyssé, A. Mokrani, C. Demangeat, J. Dorantes-Dávila, A. Vega, A. Rubio y L.C. Balbás
24. *21st Annual Symposium "Electronic Structure of Solids" and 75th WE-Heraeus-Seminar*  
Gaußig, Dresden, Alemania, 11-15 Marzo de 1991.  
CONFERENCIA INVITADA
25. *II Reunión Nacional sobre Física de Micropartículas*  
Universidad de Valladolid, Valladolid, 6-8 Mayo de 1991.  
CONFERENCIAS INVITADAS (2)
26. *XIII International Symposium on Molecular Beams*  
El Escorial, Madrid, 2-7 Junio de 1991.  
COMUNICACIÓN / POSTER.  
- *Non-Local Approximation to the Exchange and Kinetic Energy Functionals. Applications to Metallic Clusters*. M.D. Glossman, L.C. Balbás, A. Rubio y J.A. Alonso
27. *ICM*.  
Edimburgo, 2-6 Septiembre 1991.  
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- *Stepped Fe(001) Surface Magnetism*. A. Vega, A. Rubio, L.C. Balbás, J. Dorantes-Dávila, A. Mokrani, C. Demangeat y H. Dreyssé
28. *4th International Conference on the Applications of Density Functional Theory in Chemistry and Physics*.  
Centro Stefano Franscino, Monte Verità, Suiza, 23-27 Septiembre de 1991.  
POSTER.  
- *Non-Local Approximation to the Exchange and Kinetic Energy Functionals. Applications to Atoms*. M.D. Glossman, L.C. Balbás, A. Rubio y J.A. Alonso
29. *23 Reunión Bienal de la Real Sociedad Española de Física*.  
Universidad de Valladolid, Valladolid, 23-27 Septiembre de 1991.  
COMUNICACIÓN ORAL.  
- *Non-Local Approximation to the Exchange and Kinetic Energy Functionals. Applications to Metallic Clusters*. M.D. Glossman, A. Rubio, Ll. Serra, L.C. Balbás y J.A. Alonso  
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- *Magnetism of Stepped Surface and Interface*. A. Vega, A. Rubio, L.C. Balbás, J. Dorantes-Dávila, H. Dreyssé, C. Demangeat y A. Mokrani
30. *Workshop on "Dynamical Response of the Valence Gas in Simple Metal Systems"*  
Varenna, Italia, 11-16 Mayo de 1992.  
CONFERENCIA INVITADA.
31. *Sanibel Symposia*  
14-21 Marzo de 1992. Universidad de Florida.  
POSTER  
- *Non Local Exchange and Kinetic Energy Density Functional for Electronic Systems*. M.D. Glossman, L.C. Balbás, A. Rubio y J.A. Alonso
32. *Adriatico Research Conference on "Clusters and Fullerenes"*  
International Centre for Theoretical Physics. Trieste, Italia, 23-26 Junio de 1992.  
POSTER.  
- *Electronic and Geometrical Effects in the Photoabsorption Cross Sections of Sodium Clusters Beyond the Local Density Approximation and Jellium Model* A. Rubio, L.C. Balbás y J.A. Alonso

33. *6th International Symposium on Small Particles and Inorganic Clusters (ISSPIC-6)*  
University of Chicago, Chicago, Illinois, USA, 16-22 de Septiembre de 1992.  
COMUNICACIONES / POSTERS (4).  
- *Microscopic Study of the Dipole Surface Response in Large Potassium Cluster Ions.* A. Rubio y Ll. Serra  
- *Photoabsorption Cross Sections of Sodium Anion Clusters: Electronic and Geometrical Effects Beyond the Local Density Approximation and Jellium Model.* A. Rubio, L.C. Balbás y J.A. Alonso  
- *Electronic Properties of Very Large Sodium Clusters Using a Non-Local Approximation to the Exchange and Kinetic Energy Functionals.* M.D. Glossman, A. Rubio, L.C. Balbás, J.A. Alonso y Ll. Serra  
- *Collective Excitations of Embedded Potassium Clusters.* Ll. Serra y A. Rubio
34. *Density Functional Theory and its Applications, Profesor March's 65 Birthday.*  
Oxford, Inglaterra, 16-18 Septiembre de 1992.  
CONFERENCIA INVITADA  
- *Density Functional Calculation of the Photoabsorption Spectrum of Simple Metal Clusters: Beyond the Local Density Approximation and Jellium Model.* J.A. Alonso, A. Rubio y L.C. Balbás
35. *Sixth International Workshop on Computational Condensed Matter Physics*  
Trieste, Italia, 11-13 Enero 1993  
POSTER  
- *Non-local Exchange and Local Coulomb Correlation Energy Density Functionals for Finite Many-Electron Systems.* N.A. Cordero, O.V. Gritsenko, A. Rubio, L.C. Balbás y J.A. Alonso
36. *Workshop on Wide Gap Semiconductors*  
Lawrence Berkeley Laboratory. Berkeley, California, USA, 19 Febrero 1993.  
ASISTENCIA.
37. *March 1993 American Physical Society Meeting*  
Seattle, Washington, USA, 22-26 Marzo 1993.  
COMUNICACIÓN ORAL.  
- *Electronic Structure of AlN, GaN and AlN/GaN superlattices.* A. Rubio, J.L. Corkill y M.L. Cohen
38. *"Theory of Atomic and Molecular Clusters", TAMC-1*  
Leer, Alemania. 13-18 Junio 1993.  
POSTER y COMUNICACIÓN ORAL.  
- *Optical Response of  $Li_xNa_{N-x}$  ( $0 \leq x \leq N = 8, 20$ ) Bimetallic Clusters and of  $Na_8Zn$  and  $Na_9X$  ( $X = F, Cl, Br$ ) Doped Clusters.* L.C. Balbás, A. Rubio y M.B. Torres
39. *2nd International Conference on Atomic and Nuclear Clusters'93*  
Santorini, Grecia Julio 1993.  
POSTER y COMUNICACIÓN ORAL.  
- *Calculated Photoabsorption Spectra of  $Li_xNa_{n-x}$  ( $x < n = 8, 20$ ) and of  $Na_8Zn$  Clusters.* L.C. Balbás, A. Rubio y M.B. Torres
40. *NATO Advanced Study Institute on Density Functional Theory*  
Il CIOCO, Tuscany, Italia. 16-27 Agosto 1993.  
POSTER.  
- *Interconfigurational Energies Using a Weighted-Density Exchange and a Local-Density Coulomb Correlation Functional.* N.A. Cordero, O.V. Gritsenko, A. Rubio, L.C. Balbás y J.A. Alonso
41. *5th International Conference on the Applications of the Density Functional Theory in Chemistry and Physics*  
Como, Italia. 13-16 Septiembre 1993  
COMUNICACIÓN ORAL.  
- *First Ionization Potential of Atoms Calculated with Novel Exchange and Correlation Functionals.* N.A. Cordero, O.V. Gritsenko, A. Rubio, L.C. Balbás y J.A. Alonso
42. *24 Reunión Bienal de la Real Sociedad Española de Física*  
Jaca, 26-30 Septiembre de 1993.  
POSTERS (2)  
- *Propiedades Ópticas del Met-Car  $Ti_8C_{12}$ .* A. Rubio, J.A. Alonso y J.M. López  
- *Optical Response of Bimetallic and Doped Alkali Clusters.* L.C. Balbás, A. Rubio y M.B. Torres

43. *El-Sayed Symposium*. University of California at Los Angeles  
Los Angeles, USA. 5-6 Noviembre 1993.  
POSTER y COMUNICACION ORAL.  
- *Metallic-Ionic Phase Separation on the Nanoscale*. C.F. Fagerquist, D.K. Sensharma, T.S. Ahmadi, M.A. El Sayed., A. Rubio y M.L. Cohen
44. *March 1994 American Physical Society Meeting*  
Pittsburgh, PA, USA, 21-25 Marzo 1994.  
POSTER  
- *Electronic and Structural Properties of BN Nanotubes*. A. Rubio, X. Blase, S.G. Louie y M.L. Cohen
45. *"Quantum Theory of Real Materials". Symposium in Honor of Professor Marvin L. Cohen's 60th Birthday*  
13 Agosto 1994. Lawrence Berkeley Laboratory, University of California at Berkeley. USA.  
POSTER  
- *New Nanotubules of Graphitic  $B_xC_yN_z$* . Y. Miyamoto, X. Blase, A. Rubio, S.G. Louie y M.L. Cohen
46. *MRS (Materials Research Society)*  
28-Noviembre 2-Diciembre 1994, Boston, Massachusetts, USA.  
CONFERENCIA INVITADA  
- *A Real-Space Formalism for Calculation of Dynamical Screening in Extended Systems*. X. Blase, A. Rubio, S.G. Louie y M.L. Cohen
47. *Seventh International Workshop on Computational Condensed Matter Physics: "Total Energy and Force Methods"*  
International Centre for Theoretical Physics. Trieste, Italia, 11-15 Enero 1995.  
POSTER.  
- *Mixed Space Formalism for the Dielectric Screening*. A. Rubio, X. Blase, S.G. Louie y M.L. Cohen
48. *March 1995 American Physical Society Meeting*  
20-24 Marzo 1995, San Jose, California, USA.  
COMUNICACIONES ORALES (5)  
- *Ab-initio Calculations of the Structural Phase Transitions for ZnTe and CdTe*. M. Côt'e, A. Rubio, O. Zakharov y M.L. Cohen  
- *Synthesis of  $B_xC_yN_z$  Nanotubules*. Z. Weng-Sieh, K. Cherry, N.G. Chopra, X. Blase, Y. Miyamoto, A. Rubio, M.L. Cohen, R. Gronsky, S.G. Louie y A. Zettl  
- *A Mixed-Space Formalism for the Dielectric Response in Extended Systems*. X. Blase, A. Rubio, S.G. Louie y M.L. Cohen  
- *Stability and Band Gap Constancy of BN Nanotubes*. S.G. Louie, X. Blase, A. Rubio y M.L. Cohen  
- *Alkali Doped Nanotubes: Cohesion and Electronic Properties*. A. Rubio, Y. Miyamoto, X. Blase, S.G. Louie y M.L. Cohen
49. *III Reunión de Materiales Avanzados: Nanotecnologías*  
5-Abril- 5-Mayo 1995, E.T.S. Ingenieros Industriales. Valladolid.  
ORGANIZADOR y CONFERENCIA INVITADA
50. *First-Principle Theory of Polarization, Fields and Currents in Insulators*  
Centre Europeen de Calcul Atomique et Moleculaire (CECAM). Lyon, Francia, 10-13 Julio 1995.  
CONFERENCIA INVITADA
51. *E.P.S.I. Workshop*  
Università degli Studi di Roma "Tor Vergata", Dipartimento di Fisica. Roma, Italia. 27-30 Septiembre 1995.  
CONFERENCIA INVITADA
52. *NAMITECH: "Nanotubes for Microstructure Technology"*  
Onera, Châtillon, France. 13 Mayo 1996. PRESENTACION INVITADA.
53. *8th International Symposium on Small Particles and Inorganic Clusters (ISSPIC-8)*  
University of Copenhagen, Copenhagen. Dinamarca. 1-6 Julio 1996.  
POSTERS (5)  
- *Thermal Behaviour of Small Carbon Clusters and Fullerenes*. M.J. López, P.A. Marcos, A. Rubio y J.A. Alonso  
- *A First Principle Calculation of the Dipole Moments of Small Semiconductor Clusters*. A. Rubio, L.C. Balbás

y J.L. Martins

- *Electronic Structure, Electron Affinity and Magnetism of Titanium Clusters*. J. Izquierdo, M.B. Torres, A. Vega, A. Rubio y L.C. Balbás

- *Electric and Magnetic Dipole Response of Doped Clusters*. M.B. Torres, A. Rubio y L.C. Balbás

- *Optical Response of Small Ag Cluster Ions*. Ll. Serra y A. Rubio

54.  $\psi_k$  Network Conference: "Ab-initio (from Electronic Structure) Calculation of Complex Processes in Materials" Schwäbisch Gmünd, Alemania. 18-21 Septiembre 1996.

CONFERENCIA INVITADA

55. NATO Advanced Research Workshop Nanowires

Madrid, España. 23-27 Septiembre 1996

CONFERENCIA INVITADA

56. EXCAM Workshop: "Electronic Exchange and Correlation in Advanced Materials

Ecole Polytechnique, Palaiseau, Paris. 26-28 Septiembre 1996.

CONFERENCIAS INVITADAS (2)

57. International Workshop on the Current Problems in Condensed Matter: Theory and Experiments (Morelos, México) 5-9 Enero 1997.

CONTRIBUCIÓN ORAL

- *Theoretical Study of the Collective Excitations of the Endohedral Clusters  $Na_N@C_{780}$* . J.M. Cabrera-Trujillo, R. Pis Díez, J.A. Alonso, M.J. López, M.P. Iñiguez y A. Rubio

58. NAMITECH Workshop: "Nanotubes for Microstructure Technology"

Universidad de Valladolid, España. 17-21 Febrero 1997.

ORGANIZADOR, CHAIRMAN y CONFERENCIA INVITADA (2)

59. "International Winterschool on electronic Properties of Novel Materials: Molecular Nanostructures"

Hotel Sonnalp, Kirchberg, Austria. 1-8 Marzo 1997.

PARTICIPACION INVITADA.

60. 1997 American Physical Society Meeting

17-21 Marzo 1997, Kansas City, Kansas, USA.

COMUNICACIÓN ORAL

- *Defect-Induced Metallization of Carbon Nanotubes*. V.H. Crespi, M.L. Cohen y A. Rubio

61. ACS, Division of Computers in Chemistry, Symposium on Recent Developments in Molecular Simulations Using Density Functional Theory

San Francisco, USA. 13-17 Abril 1997

CONFERENCIA INVITADA

- *Bimetallic Clusters of Interest for Liquid Alloys*. J.A. Alonso, L.M. Molina, M.J. López y A. Rubio

62. Symposium on Density Functional Theory and Applications

Duke University, Durham, North Carolina, USA. 3-7 Junio 1997

CONFERENCIA INVITADA

- *Electronic Structure of Pure and Mixed Lead Clusters*. J.A. Alonso, L.M. Molina, M.J. López y A. Rubio

63. International Conference "Physics of Clusters: Clusters in Plasma and Gases"

Puschino, Rusia, 17-23 Agosto 1997

CONFERENCIA INVITADA

- *Thermal Road for Fullerene Annealing*. M.J. López, P.A. Marcos, A. Rubio y J.A. Alonso

64. European Research Conference on "Chemistry and Physics of Multifunctional Materials"

Espinho, Portugal, 6-11 Septiembre 1997

POSTERS (2)

- *Thermal Road for Fullerene Annealing*. M.J. López, P.A. Marcos, A. Rubio y J.A. Alonso

- *Tight-Binding NVT Molecular Dynamics Simulation of Nanotubes*. E. Hernández, C. Goze y A. Rubio

65. CECAM Workshop on "Excited Electrons in Molecules, Solids and Atoms"

Lyon, Francia, 8-10 Septiembre 1997

CONFERENCIA INVITADA

66. *EXCAM Workshop "Electronic Exchange and Correlation in Advances Materials"*  
Lyon, Francia, 11-12 Septiembre 1997  
CHAIRMAN
67. *XXVI Reunión Bienal RSEF*  
Las Palmas, Gran Canaria, 29 Septiembre- 3 Octubre 1997  
POSTER  
- *Dinámica Molecular de Agregados Metálicos en Superficies*. F.J. Palacios, M.P. Iñiguez, M.J. López, A. Rubio y J.A. Alonso
68. *Micropscopy of Nanotubular Structures Joint Workshop: NAMITECH and NEDO Networks*  
Institut des Matériaux, Université de Nantes, Nantes, Francia. 27-30 Octubre 1997.  
CONFERENCIA INVITADA y COORDINADOR  
- *Theoretical Investigation of the Elastic Properties of Single-Wall Nanotubes*. E. Hernández, C. Goze y A. Rubio.
69. *"International Winterschool on electronic Properties of Novel Materials: Molecular Nanostructures"*  
Hotel Sonnalp, Kirchberg, Austria. 28-Febrero 7-Marzo 1998.  
POSTER.  
- *Tight Binding Calculation of the Elastic Properties of Single Wall Nanotubes*. E. Hernández, C. Goze y A. Rubio
70. *March 1997 American Physical Society Meeting*  
16-20 Marzo 1998, Los Angeles, CA, USA.  
COMUNICACIÓN ORAL  
- *Theoretical Investigation of the Elastic Properties of Single-Wall Nanotubes*. E. Hernández, C. Goze, P. Bernier y A. Rubio.  
- *Ab Initio Studies of Tin and Lead Clusters*. B. Wang, M.J. Stott, L.M. Molina, M.J. López, A. Rubio y J.A. Alonso.
71. *NAMITECH Workshop: "Nanotubes for Microstructure Technology"*  
CRMD, Orleans, Francia. 9-10 Abril 1998.  
CHAIRMAN, COORDINADOR y CONFERENCIA INVITADA (1)
72. *IBER98: III Iberian Joint Meeting on Atomic and Molecular Physics*  
4-7 Mayo 1998, Mira, Portugal.  
COMUNICACIÓN ORAL  
- *Electronic Structure of Clusters Formed by Pb and Alkali Atoms*. J.A. Alonso, L.M. Molina, M.J. López, A. Rubio y M.J. Stott.
73. *Workshop on Computational Chemistry*  
18-20 Junio 1998, Miraflores de la Sierra, Madrid.  
COMUNICACIÓN ORAL  
- *Electronic Structure of Na-Pb Clusters and of Solids Containing Those Clusters*. J.A. Alonso, L.M. Molina, M.J. López, A. Rubio y M.J. Stott.
74. *International Conference on Science and Technology of Synthetic Metals (ICSM'98)*  
12-18 Julio 1998, Montpellier, Francia.  
(POSTERS 2)  
- *Elastic and Mechanical Properties of Carbon Nanotubes*. C. Goze, L. Vaccarini, L. Henrard, P. Bernier, E. Hernández y A. Rubio  
- *What is the Chirality of the Carbon Singlewalled Nanotubes ?*. L. Henrard, A. Rubio, P. Senet, E. Hernández, C. Journet, C. Goze, L. Vaccarini, A. Loiseau y P. Bernier.
75. *14-International Vacuum Congress (IVC-14) and 10<sup>th</sup>-International Conference on Solid Surfaces (ICSS-10)*  
31-Agosto 4-Septiembre 1998, Birmingham, UK.  
COMUNICACIÓN ORAL  
- *Interface and bulk effects in the transmission of low energy electrons through thin, wide-gap insulating films on semiconductors*. J.E. Ortega, F.J. García de Abajo, P.M. Echenique, J. Manke, T. Kalka, M. Dähne, D. Ochs, S.L. Molodtsov, C. Laubschat y A. Rubio

76. *9th International Symposium on Small Particles and Inorganic Clusters (ISSPIC-9)*  
1-5 Septiembre 1998, Palias de Beaulie, Lausanne, Suiza.  
POSTERS (2)  
- *Building Alkali-Pb Alloys from Clusters*. J.A. Alonso, L.M. Molina, M.J. López, A. Rubio y M.J. Stott.  
- *Structural and Thermal Properties of Silicon-Doped Fullerenes*. P.A. Marcos, M.J. López, A. Rubio y J.A. Alonso.
77. *EXCAM Workshop: "Spectroscopy of Electronic Excitations in Materials"*  
Universidad de Valladolid, Valladolid, España. 7-9 Septiembre 1998.  
ORGANIZADOR y CHAIRMAN.
78. *CECAM Workshop on "Simulation of Carbon and composite  $B_xC_yN_z$  Nanotubes"*  
Lyon, Francia, 1-3 Septiembre 1998  
CONFERENCIAS INVITADAS (2).
79. *Nanotechnology in Carbon and Related Materials*  
September 9-11th 1998, University of Sussex at Brighton, U.K.  
CONFERENCIAS INVITADAS (2)  
- *Designing compound nanotubes by first-principles computations*. Y. Miyamoto, E. Hernandez, A. Rubio y B. D. Yu.  
- *Tight-Binding Calculation of the Elastic Properties of Single-Wall Nanotubes*. E. Hernandez, C. Goze, P. Bernier y A. Rubio
80. *XLI Congreso Nacional de Física*  
Universidad Autónoma de San Luis Potosí, México, 26-30 Octubre 1998.  
COMUNICACIÓN  
- *Excitaciones Colectivas de la Cebolla de Carbón*. E.O. Berlanga-Ramírez, J.M. Cabrera-Trujillo, J.A. Alonso, A. Rubio y M.J. López.
81. *MRS Fall Meeting*.  
Boston, Estados Unidos, 30-Noviembre al 4-Diciembre 1998.  
COMUNICACIÓN ORAL.  
- *Elastical and Mechanical Properties of Carbon Nanotubes*. L. Vaccarini, C. Goze, P. Bernier, E. Hernández y A. Rubio.
82. *March 1999 American Physical Society Meeting*  
Atlanta, Georgia, USA, 22-26 Marzo 1999.  
COMUNICACIONES ORALES (5).  
- *Spectroscopic Properties and STM Images of Carbon Nanotubes*. A. Rubio  
- *Structural, Elastic and Vibrational Properties of Carbon Nanotubes*. D. Sánchez-Portal, E. Artacho, J.M. Soler, A. Rubio y J.M. Soler  
- *GW Self-Energy Calculations Using the Space-Time Method*. L. Steinbeck, M.M. Rieger, A. Rubio, I.D. White, H.N. Rojas y R.W. Godby  
- *Interface and Bulk Effects in the Transmission of Low Energy Electrons Through Thin, Wide-gap Insulating Films on Semiconductors*. J.E. Ortega, F.J. García de Abajo, P.M. Echenique, J. Manke, T. Kalka, M. Dähne, D. Ochs, S.L. Molodtsov, C. Laubschat y A. Rubio  
- *Junctions in Doped Semiconductor Carbon Nanotubes*. A. Rubio, V. Crespi y P. Lammert
83. *NAMITECH Workshop: "Nanotubes for Microstructure Technology"*  
St. Patrick's College, Maynooth (Dublin), Irlanda. 8-11 Abril 1999.  
CHAIRMAN y COORDINADOR.
84. *Física Estadística '99 (IX Congreso)*  
Instituto de Física de Cantabria. Santander 6-8 Mayo (1999)  
CONFERENCIA INVITADA
85. *Conferencia de Dispositivos Electrónicos 1999*  
Madrid, 10-11 Junio (1999)  
POSTER  
- *Effect of Silicon Bonds on Channeling Implant Simulations*. J. Hernández, M. Jaraiz, J. Arias, L. Bailón, J. Barbolla y A. Rubio

86. *ACSIN-5: Atomically Controlled Surfaces, Interfaces and Nanostructures*  
Aix en Provence, Francia. 6-9 de Julio 1999  
COMUNICACION ORAL  
- *Electronic Structure of Nanostructures Based on Carbon Nanotubes*. N. Zabala, M.J. Puska, A. Rubio y R.M. Nieminen.
87. *Imboron X- An international Conference on the Chemistry of Boron*  
University of Durham, UK, 11-15 Julio (1999)  
POSTER  
- *Ab-initio Study of Boron-Hydrogen Spheres*. I. Boustani, A. Rubio y J.A. Alonso
88. *NANOTUBE-99, International Workshop on the Science and Application of Nanotubes*  
East Lansing, Michigan, USA, July 24-27, (1999)  
CONFERENCIA INVITADA  
- *Simulations of STM Images of Carbon Nanotubes*. Ph. Lambin, V. Meunier y A. Rubio.
89. *Fullerenes'99: A workshop on Nanotubes and Fullerene Chemistry*  
Château Bonas, France. 29-Agosto al 2-Septiembre 1999  
CONFERENCIA INVITADA
90. *NanoteC99: Nanotechnology in Carbon and Related Materials*  
University of Sussex, Brighton UK. 8-10 Septiembre 1999  
CONFERENCIA INVITADA
91. *XXVII Reunión Bienal de la Real Sociedad Española de Física*  
Valencia, 20-24 Septiembre 1999.  
POSTER  
- *Estudio ab initio de la estabilidad y propiedades de agregados mixtos Plomo-alkalino en aleaciones sólidas*. L. M. Molina, J. A. Alonso, M. J. López, A. Rubio y M. J. Stott
92. *III International Symposium on Theory of Atomic and Molecular Clusters*.  
Berlin, 3-5 Octubre 1999.  
CONFERENCIA INVITADA  
- *Ab initio modelling of Alkali-Pb alloys from clusters*. J. A. Alonso, L. M. Molina, M. J. López, A. Rubio, y M. J. Stott
93. *II Congress of the International Society for Theoretical Chemical Physics*  
Ciudad de Mexico, 8-13 Noviembre 1999  
POSTER  
- *Theoretical study of the collective electronic excitations of  $C_{60}NaC_{240}$* . E. Berlanga-Ramírez, J. M. Cabrera-Trujillo, J. A. Alonso, A. Rubio
94. *MRS Fall Meeting*  
Symposium: Computational Approaches to Predicting the Optical Properties of Materials  
Boston, Estados Unidos, 30-Noviembre al 3-Diciembre 1999.  
CONFERENCIA INVITADA y COMUNICACION ORAL  
- *Inelastic deformations in multiwalled carbon nanotubes*. D. Tekleab, R. Czerw, A. Rubio, P.M. Ajayan y D. Carroll
95. *"International Winterschool on electronic Properties of Novel Materials: Molecular Nanostructures"*  
Hotel Sonnalp, Kirchberg, Austria. 4-11 Marzo 2000.  
PARTICIPACION INVITADA.  
- *Theoretical estimates of the electronic transport features in carbon nanotubes*. A. Rubio and S. Roche  
- *Density Functional Study of Absorption of Lithium and Molecular Hydrogen on Graphene Sheets*. J.S. Arellano, L.M. Molina, M.J. López, A. Rubio y J.A. Alonso.
96. *March 2000 American Physical Society Meeting*  
Minneapolis MN, USA, 20-24 Marzo 2000.  
COMUNICACIONES ORALES (3).  
- *Local Density of States of Kinked Multiwalled Nanotubes*. D. Tekleab, R. Czerw, A. Rubio, P.M. Ajayan y D. Carroll  
- *Ab initio molecular dynamics simulations of melting in the NaSn alloy*. L.M. Molina, J.A. Alonso, M.J. López,

- A. Rubio y M.J. Stott  
- *Self-energy of low energy quasielectrons and quasiholes in graphite*. M.A. Cazalilla, A. Rubio y P.M. Echenique
97. *Psi-k 2000 Conference on "Ab Initio (from Electronic Structure) Calculations of Complex Processes in Materials"*  
Schwäbisch Gmünd, Alemania 22-26 Agosto 2000  
CONFERENCIA INVITADA
98. *Nanotubes 2000: 3<sup>eme</sup> Colloque Annual GDR-1752 CNRS*  
Toulouse, 6-8 Noviembre 2000  
COMUNICACIÓN ORAL  
-*Propriétés Vibrationnelles des Faisceaux de Nanotubes Finis et Infinis: les Modes Radiaux et leur Derivés*. L. Henrard, V. Popov and A. Rubio
99. *International Symposium on Nanonetwork Materials: Fullerenes, Nanotubes and Related Systems (ISNM2001)*  
Kamakura, Japan 15-18 Enero 2001  
COMUNICACIÓN ORAL  
-*Electronic transport in multiwall carbon nanotubes* F. Triozon, A. Rubio, D. Mayou y S. Roche
100. *ICAS 2001: International Conference on Atomic Collisions*  
Paris, Julio 2001.  
COMUNICACIÓN ORAL  
-*Stopping power of aluminum oxide* I. Gurtubay, T. Pitarke y A. Rubio
101. *NT01*  
Postdam, Alemania 20-26 Julio 2001  
3 POSTERS, ORGANIZADOR  
*Transformation of Single-Wall carbon nanotube ropes into multiwall carbon nanotubes* M.J. López, A. Rubio, K. Metenier, S. Bonamy  
*Multiwall carbon nanotubes as non-ballistic conductors* S. Roche, F. Triozon, A. Rubio  
*Ab-initio calculation of the absorption and energy-loss spectra of a bundle of carbon nanotubes*, A.G. Marinopoulos, L. Reining, A. Rubio y V. Olevano
102. *Nanotec01*  
Brighton, UK. 29 Agosto-1 Septiembre 2001  
COMUNICACIÓN ORAL  
-*Influence of packing on the vibrational properties of infinite and finite bundles of carbon nanotubes* L. Henrard, V. Popov, A. Rubio
103. *Nanotubes 2001: 4<sup>eme</sup> Colloque Annual GDR*  
Nantes, Francia, 1-4 Octubre 2001  
COMUNICACIÓN ORAL  
*Influence des interactions intertubes sur les propriétés vibrationnelles de nanotubes de carbone mono- et multi-feuillets* L. Henrard, V. Popov, A. Rubio
104. *International Conference on the Applications of Density Functional Theory to Chemistry and Physics*  
El Escorial, 10-14 Septiembre 2001.  
POSTERS (3) AND CONFERENCIA INVITADA  
-*Photoelectron spectra from TDDFT* H. Appel, M. Marques, A. Rubio and E.K.U. Gross. -*Optical response of Ni<sub>2</sub> and the metastable species Ni<sub>2</sub><sup>2+</sup>*, A. Bol, R. Pis-Diez, A. Rubio and J.A. Alonso.
105. *21<sup>st</sup> Werner Brandt Workshop on Penetration Phenomena: Atoms and Molecules at surfaces*  
San Sebastián, España, 17-18 Septiembre 2001  
CONFERENCIA INVITADA  
*Screening and quasiparticle lifetimes in bulk metals and their surfaces* E. Chulkov, V.M. Silkin, A. Rubio, V.P. Zhukov y P.M. Echenique
106. *XLIV Congreso Nacional de Física de la Sociedad Mexicana de Física*  
COMUNICACIÓN ORAL  
-*Litio intercalado en grafito, algunos resultados con teoría de funcionales de la densidad*, J.S. Arellano, L.M. Molina, M.J. López, A. Rubio y J.A. Alonso.



107. *Tsukuba Symposium on Carbon Nanotube: CNT10*  
Tsukuba, Japon (3-5 Octubre 2001)  
CONFERENCIA INVITADA  
-*Onset of nanotube decay under extreme thermal and electronic excitations* Y. Miyamoto, S. Berber, M. Yoon, A. Rubio y D. Tománek
108. *Workshop: Total Energy Methods in Computational Condensed Matter*  
La Laguna, Tenerife, España. (10-12 Enero 2002) CONFERENCIA INVITADA  
-*Effects of long-range interactions in the absorption and loss spectra of finite and infinite systems*, L. Reining, S. Botti, A.G. Marinopoulos, V. Olevano, F. Sottile, N. Vast, A. Rubio y G. Onida.
109. *Encuentros sobre Fronteras de la Ciencia*  
Salamanca, 19-20 Febrero 2002. INVITADO/MODERADOR.
110. *March 2002 American Physical Society Meeting*  
18-22 Marzo 2002, Indianapolis, Indiana, USA.  
COMUNICACIONES ORALES (3)  
-*Laser induced inverse Landau damping in metallic nanoparticles* M.E. Garcia, A. Castro, J.A. Alonso y A. Rubio  
-*Excited state dynamics of carbon nanotubes with defects: a time-dependent Kohn-Sham approach* Y. Miyamoto, S. Berber, M. Yoon, D. Tomanek y A. Rubio  
-*Excitonic effects in solid described by time-dependent density-functional theory* V. Olevano, L. Reining, A. Rubio y G. Onida.
111. *ICPS: 26th International Conference on the Physics of Semiconductors -Pressure and temperature investigation of Raman modes in CuI* J. Serrano, M. Cardona, B. Weinstein, T. Ritter y A. Rubio
112. *CECAM Workshop: Open Software for Microscopic Calculations*  
Lyon, Francia, 19-21 Junio 2002  
CONFERENCIA INVITADA  
-*Octopus: a first-principles tool for electron-ion dynamics*, M.A.L. Marques, A. Castro, G.F. Bertsch y A. Rubio
113. *International Workshop: Towards atomic scale- and time- resolution at interfaces*  
San Sebastián/Donostia 1-5 Julio 2002  
CONFERENCIA INVITADA Y DIRECTOR  
-*Optical Properties of nanostructures: a first-principle approach*, A. Castro, M.A.L. Marques, G.F. Bertsch y A. Rubio
114. *NT02*  
Boston College, Boston, USA 6-11 Julio 2002  
CONFERENCIA INVITADAS (2) y POSTER  
-*Electronic and Structural Properties of BN tubes*, L. Wirtz, R. Arenal de la Concha, A. Loiseau y A. Rubio  
-*Computational Diagnosis of Defective Nanotubes: Stability with Respect to Thermal and Optical Perturbations* Y. Miyamoto, S. Berber, M. Yoon, A. Rubio y D. Tomanek  
-*Magnetotransport and persistent currents in carbon nanotube based materials* S. Roche, S. Latil, A. Rubio y R. Saito
115. *11th International Symposium on Small Particles and Inorganic Clusters (ISSPIC-11)*  
1-5 Septiembre 2002, Strasbourg, Francia.  
POSTERS (1)  
-*Interaction of molecular and atomic hydrogen with single wall carbon nanotubes*, J.A. Alonso, J.S. Arellano, L.M. Molina, A. Rubio and M.J. López
116. *VIIIes Journées de la Matière Condensée*  
27-30 Agosto 2002, Marsella, Francia.  
CONTRIBUCIÓN ORAL  
-*Synthèse de BN-NTs et premières études des propriétés vibrationnelles*, R. Arenal de la Concha, A. Loiseau, J.-Y. Mevellec, A. Rubio, A. Vlandas, O. Stéphan, J.-L. Cochon, J. Thibault
117. *CECAM PSI-k Workshop: "Ab initio Theoretical Approaches to the Electronic Structure and Optical Spectra of Materials"*  
Lyon, Francia, 22-26 Septiembre 2002  
CHAIRMAN.

118. *ICORP Nanotubulites project*  
Final meeting 11-13 October 2002, Gif sur Yvette, France  
POSTER  
*-Synthesis and vibrational properties of Boron Nitride nanotubes*, R. Arenal de la Concha, L. Wirtz, A. Loiseau, A. Rubio, J.-Y. Mevellec, A. Vlandas, S. Lefrant, O. Stéphan, and J. Thibault
119. *43 Sanibel Symposium*  
Florida , USA 22 Febrero-1 Marzo 2003  
POSTER *DFT ab initio study of the interaction of molecular and atomic hydrogen with (5,5) and (6,6) single wall carbon nanotubes*, J.S. Arellano, L.M. Molina, A. Rubio, M.J. Lopez and J.A. Alonso
120. *March 2003 American Physical Society Meeting*  
March 3-7, Austin, Texas  
CONTRIBUTED TALK  
*Photo-induced cleaning of oxidized carbon nanotubes*, Y. Miyamoto, A. Rubio and D. Tomanek
121. *International Winterschool on Electronic Properties of Novel Materials Molecular Nanostructures (IWEPNM2003)*  
March 8-15 (2003), Kirchberg/Tirol, Austria CONFERENCIANTE INVITADO Y POSTERS (3)  
*-Synthesis and vibrational properties of Boron Nitride nanotubes*, R. Arenal de la Concha, L. Wirtz, A. Loiseau, A. Rubio, J.-Y. Mevellec, A. Vlandas, S. Lefrant, O. Stéphan, and J. Thibault  
*-Electronic structure and optical properties of heteronanotubes: MWNBNNT and B-doped SWNT* E. Borowiak-Palen, G. Fuentes, F. Hasu, A. Kukovecz, L. Wirtz, A. Rubio, M. Knupfer, A. Grafft, R.J. Kalenczuk, T. Pichler and J. Fink.  
*-Band structure of boron substituted carbon nanotubes: implications for optical spectroscopy*, L. Wirtz and A. Rubio
122. *"Nanotechnology" Symposium (EMT103) of the SPIE's "Microtechnologies for the New Millenium 2003"*  
Maspalomas, Gran Canaria, Spain 19-21 Mayo 2003.  
CONFERENCE CHAIR, 4 CONTRIBUTED TALKS  
*Optical and vibrational properties of BN nanotubes*. L. Wirtz and A. Rubio  
*Deformations and Thermal Stability of Carbon Nanotube Ropes*, M.J. López, A. Rubio and J.A. Alonso  
*Interaction of molecular and atomic hydrogen with single wall carbon nanotubes* , J.A. Alonso, J. Arellano, L.M. Molina, A. Rubio and M.J. López  
*Local electronics and vibrational properties of singlewall carbon nanotubes in contact with metals*. L. Vitali, L. Wirtz, A. Rubio and K. Kern
123. *NT03*, Seoul, Korea 7-11 July 2003  
CONTRIBUTED TALK  
*Ultra-Fast Nanotube De-Oxidation Driven by Electronic Excitation*, Y. Miyamoto, N. Jinbo, A. Rubio and D. Tomanek
124. *Nanomaterials and Nanotechnologies 2003 (NN2003)*  
CONTRIBUTED TALK  
*Analysis of the behaviour of single wall carbon nanotubes under tensile stress by direct HRTEM observation*, M. José-Yacamán, H.E. Troiani, G.A. Camacho-Bragado, M. Miki.Yoshida, A. Rubio and M.L.A. Marques
125. *COLA'03: 7th International Conference on Laser Ablation*, Crete, Greece 5-10 October 2003  
CONTRIBUTED TALK  
*- Simulations of laser ablation of carbon nanotubes: diameter specific purification*, A.H. Romero, H. Jeschke, A. Rubio and M.E. Garcia.
126. *TNT2003 "Trends in Nanotechnology"* Salamanca, 15-19 Septiembre 2003  
CHAIRMAN/ CONFERENCIANTE INVITADO
127. *International Winterschool on Electronic Properties of Novel Materials Molecular Nanostructures (IWEPNM2004)*  
March 6-13 (2004), Kirchberg/Tirol, Austria CHAIRMAN/CONFERENCIANTE INVITADO y POSTER  
*-Gap Measuremen in single wall boron nitride nanotubes*, R. Arenal de la Concha, O. Stephan, M. Kociak, D. Taverna, A. Rubio and A. Loiseau

128. *1st Nanospain Workshop*  
Palacio Miramar, San Sebastian, 10-12 Marzo 2004  
COMUNICACION ORAL  
-*Interaction of hydrogen with carbon nanotubes*, J.A. Alonso, I. Cabria, M.J. López, J.S. Arellano, L.M. Molina, A. Rubio.
129. *NT04*  
San Luis Potosi, Mexico, 19-24 Julio 2004  
COMUNICACIONES ORAL (2)  
-*Ultrafast decay of excited carriers in carbon nanotubes: Time-dependent density functional approach*, Y. Miyamoto, A. Rubio, and D. Tomanek  
-*Electron Energy loss and resonant raman spectroscopy of single walled boron nitride nanotubes*, R. Arenal de la Concha, O. Stephan, A. Ferrarim D. Taverna, S. Reich, A. Rubio and A. Loiseau
130. *Encuentros sobre Fronteras de la Ciencia*  
Salamanca, Febrero 2005. INVITADO/MODERADOR.
131. *DFG 2005*  
Berlin, Alemania 4-9 Marzo 2005  
COMUNICACIÓN ORAL  
-*A practical scheme for quantum transport using time-dependent density functional theory*, S. Kurth, G. Stefanucci, C.O. Almbladh, A. Rubio and E.K.U. Gross
132. *International Winterschool on Electronic Properties of Novel Materials Molecular Nanostructures (IWEPNM2005)*  
March 12-19 (2005), Kirchberg/Tirol, Austria POSTER  
-*EELS study in low-loss region of individual boron nitride nanotubes*, R. Arenal de la Concha, O. Stephan, M. Kociak, D. Taverna, A. Rubio and A. Loiseau and C. Colliex.
133. *March 2005 American Physical Society Meeting*  
March 21-25, Los Angeles CA  
CONTRIBUTED TALK  
*Atomistic simulation of the laser fragmentation of single wall carbon nanotubes*, Harald Jeschke, Aldo Romero, Martin Garcia, Angel Rubio
134. *Encuentros sobre Fronteras de la Ciencia*  
Valladolid, 21-22 Febrero 2006. INVITADO/MODERADOR.
135. *March 2006 American Physical Society Meeting*  
March 13-17, Baltimore, MD  
INVITED AND CONTRIBUTED TALK  
*A time-dependent density functional theory approach for the excited state dynamics of nanostructures and biomolecules* A. Rubio  
*Real-time ab initio simulations of excited carrier dynamics in carbon nanotubes.*, Y. Miyamoto, A. Rubio, D. Tomanek
136. *Spanish Molecular Electronics Symposium, SMS2006*  
Donostia, 24 Marzo 2006. INVITED TALK  
*Combining ab initio and semi-empirical approaches for STM simulations of molecules weakly bonded to surfaces*  
M. Dubois, S. Latil, L. Scifo, B. Grévin and A. Rubio
137. *TNT2006*  
4-8 Septiembre-2006, Grenoble, France  
POSTER  
*STM induced molecular dynamics of biphenyl on Si(100): a theoretical analysis*, M. Dubois, C. Delrue and A. Rubio
138. *Encuentros sobre Fronteras de la Ciencia*  
Salamanca, 21-22 Febrero 2007. INVITADO/MODERADOR.

139. *March 2007 American Physical Society Meeting*  
Denver, Colorado, USA, 5-9 Marzo 2007.  
INVITED TALK  
*Real-time ab initio simulations of excited-state dynamics in nanostructures*, D. Tomanek, Y. Miyamoto, A. Krasheninnikov, A. Rubio COMUNICACIÓN ORAL.  
- *Optical and magnetic excitations in small transition-metal clusters using TDDFT* M. Oliveira, F. Nogueira and A. Rubio.
140. *International Winterschool on Electronic Properties of Novel Materials (IWEPNM2007)*, March 10-17 (2007), Kirchberg/Tirol, Austria  
INVITED TALK, 2 POSTERS  
- Doping dependence of the electron phonon interaction in graphite, A. Gruneis, C. Attaccalite, D. Vyalikh, A. Rubio and Th. Pichler  
- Functionalised carbon nanotubes for integrated nano-electronic sensors Y. Pouillon, A. Rubio
141. *Progress in ab initio modelling of biomolecules : towards computational spectroscopy*  
Dipartimento di Fisica Università di Roma ( Roma, 2-4 April 2007)  
INVITED TALK, POSTER AND CHAIRMAN  
- *Excited-state properties of native and size-expanded nucleobasis: a TDDFT study*, D. Varsano, A. Migliori, S. Corni, A. Rubio, A. Garbesi, R. Di Felice.
142. EP2DS-17  
Genova July 2007 <http://www.ep2ds-mss.infm.it/>  
INVITED TALK  
- *Optimal laser-control of two-dimensional nanodevices* E. Räsänen, A. Castro, J. Werschnik, A. Rubio, and E.K.U. Gross,
143. *3rd Meeting of Spanish Users of Synchrotron Radiation*  
Jaca, 8-12 Julio 2007 CONTRIBUTED TALK  
- *Vibrational properties of hexagonal Boron Nitride: Inelastic x-ray scattering and ab initio calculations*; J. Serrano, A. Bosak, R. Arenal, M. Krisch, K. Watanabe, T. Taniguchi, A. Rubio and L. Wirtz
144. *Pan American Advanced Study Institute on Electronic States and Excitations on Nanostructures*  
Zacatecas, Mexico, June 11-22, 2007  
POSTER  
Ground state and optical properties of Methylphenidate-Dexmethylphenidate using DFT y TDDFT; A.H. Romero, L.A. Espinosa L., A. Rubio
145. *12th Density Functional Theory Conference*  
Amsterdam, The Netherlands, from 26-30 August 2007  
INVITED AND CONTRIBUTED TALK
146. *12th Nanoquanta Workshop on Electronic Excitations*  
Aussois (Savoy, Rhône-Alpes), France "Paul Langevin" CNRS centre September 18-22, 2007  
CHAIRMAN, INVITED AND CONTRIBUTED TALK, POSTERS  
Defects in semiconductors and their optical spectra, M. Bockstedte, A. Marini and A. Rubio (invited)  
Structural and optical transitions of the biliverdin Chromophore, Y. Pouillon, F. Sottile, M. Gruning, X. Lopez and A. Rubio (invited)  
Transport properties in nanotubes doped with DR1 azobencene, J. Garcia-Lastra, K. Thygesen and A. Rubio  
Abinitio optical absorption spectra of native and size expanded xDNA base assemblies, D. Varsano, A. Migliore, S. Corni, A. Rubio, A. Garbesi and R. Di Felice
147. *International Conference on Silicon Carbide and related materials (ICSCRM)*  
Otsu, Japan October 14-19, 2007  
INVITED TALK  
Defects identified in SiC and their Implications M. Bockstedte, A. Marini, A. Gali, O. Pankratov, and Angel Rubio
148. *Symposium "Exact-exchange and hybrid functionals meet quasiparticle energy calculations"*  
DPG spring meeting 2008, Berlin (25-29 February 2008)

## CONTRIBUTED TALKS

Theoretical Spectroscopy of Point Defects in Semiconductors, M. Bockstedte, A. Gali, A. Marini, A. Rubio and O. Pankratov  
N. Helbig, E.K.U. Gross

149. International Winterschool on Electronic Properties of Novel Materials (IWEPNM2008), March 1-8 (2008), Kirchberg/Tirol, Austria  
INVITED TALK, 2 POSTERS  
- Unravelling the electronic structure of intercalated graphite: a key to graphene and single-wall carbon nanotubes A. Gruneis, C. Attaccalite, A. Rubio, S. Molodtsov, D. Vyalikh, W. Eberhard, J. Fink and Th. Pichler  
- Dimensionality effects in the optics of BN nanostructures: applications for optoelectronic devices, C. Attaccalite, A. Rubio, A. Marini and L. Wirtz  
- Monitoring several environmental parameters at once: multi-level modelling of carbon nanotube based sensors, Y. Poillon, J. M. García Lastra and A. Rubio.
150. Workshop on 'New horizons in modelling surface processes' at University College London, UK , 31-March-3-April (2008)  
ORAL CONTRIBUTION  
- Excess electron on ice surfaces, F. Baletto, S. Scandolo, A. Rubio, M. Bockstedte
151. Sitges Conference on "Statistical Mechanics of Molecular Biophysics"  
Sitges, Barcelona 2-6 June 2008  
ORAL CONTRIBUTION  
- An efficient new Ehrenfest approach for Born-Oppenheimer molecular dynamics based in time-dependent density functional theory, J.L. Alonso, X. Andrade, P. Echenique, F. Falceto, D. Prada-Gracia and A. Rubio
152. *NT08*  
Montpellier Francia, 29 Junio-4 Julio (2008)  
ORAL CONTRIBUTION /INVITED TALK  
- Graphite intercalation compound  $KC_8$  revisited: a key to graphene, A. Grüneis, C. Attaccalite, A. Rubio, D. Vyalikh, S.L. Molodtsov, R. Follath, J. Fink and T. Pichler  
- Optical Properties of BN nanostructures, C. Attaccalite, L. Wirtz, A. Marini and A. Rubio
153. *6th Conference on Ultrafast Surface Dynamics*  
Berlin, 20-25 July 2008  
ORAL CONTRIBUTION  
- Non-adiabatic electron-phonon decoupling in graphite, K. Ishioka, M. Kitajima, L. Wirtz, A. Rubio, and H. Petek
154. *International Workshop "Nanocarbon Photonics and Optoelectronics"*
155. *Graphene Week 2008*  
25 - 29 August 2008, ICTP-Miramare-Trieste, Italy  
POSTER  
- Electron-electron correlation in graphite and graphene, C. Attaccalite, A. Gruneis, T. Pichler and A. Rubio
156. *European Physical Society, Condensed Matter Conference*  
25-29 August 2008, Rome (Italy)  
INVITED TALK  
- Electron-electron correlation in graphite and graphene, C. Attaccalite, A. Gruneis, T. Pichler and A. Rubio
157. *13th ETSF/Nanoquanta Conference - Theoretical Spectroscopy and Quantum Transport*  
Pugnochiuso, Vieste - 23-27 September 2008  
INVITED TALK, ORAL CONTRIBUTION, POSTERS  
-Effect of impurities on the optical properties of BN nanostructure, C. Attaccalite, L. Wirtz, A. Marini and A. Rubio  
-Excess electron solvation on crystalline ice films, M. Bockstedte, F. Baletto, S. Scandolo and A. Rubio
158. *International Conference on Materials Discovery and Databases : Informatics and DFT*  
11-13 October 2008, University of Tlemcen, Oran, Algeria  
INVITED TALK  
Ab-initio band structure of graphene and graphite, C. Attaccalite, A. Gruneis, T. Pichler and A. Rubio

159. *14th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods*  
Trieste, Italy, 8 - 10 January 2009  
INVITED TALK AND POSTER  
- *Electron correlation in graphene: band structure and electron-phonon interaction from GW*  
- *Optical saturation driven by exciton confinement in molecular chains: a TDDFT study*, D. Varsano, A. Marini and A. Rubio
160. International Winterschool on Electronic Properties of Novel Materials (IWEPNM2009), March 8-14 (2009), Kirchberg/Tirol, Austria  
Invited Talk  
- Electron phonon coupling in graphene, C. Attaccalite and A. Rubio
161. *March 2009 American Physical Society Meeting*  
Pittsburgh, PA, USA, 16-20 March 2009.  
INVITED AND CONTRIBUTED TALKS  
- Incorporating Exchange-Correlation Effects in Quantum Transport through Nano-scale Junctions, K. Thygesen and A. Rubio  
- Non-linear optics and local-field factors in liquid chloroform: A time-dependent density-functional theory study, D.A. Strube, X. Andrade, A. Rubio and S. G. Louie  
- Optical spectra with spin-orbit effects on gold nanostructures, A.H. Romero, A. Castro, M. A. L. Marques, M. J. T. Oliveira and A. Rubio  
- Tailoring High-Order Harmonics: A Computational Approach Based on Time-Dependent Density-Functional Theory, A. Castro, A. Akbari, A. Rubio and E.K.U. Gross  
- Impact of the electron-electron correlation on phonon dispersion: failure of LDA and GGA DFT functionals in graphene and graphite, M. Lazzeri, C. Attaccalite, L. Wirtz, A. Rubio and F. Mauri.
162. *DPG Spring Meeting*  
Dresden, 22nd - 27th of March 2009  
CONTRIBUTED TALKS  
- Exact Kohn-Sham potential of strongly correlated systems, N. Helbig, I. Tokatly and A. Rubio  
- Trapping of electrons on ice surfaces: an ab initio study, M. Bockstedte, F. Balleto, S. Scandolo, and A. Rubio
163. *NT09*  
Beijing, China, June 21-26, 2009  
ORAL CONTRIBUTION  
- Electron-phonon coupling in graphene layers investigated by angle-resolved photoemission and inelastic x-ray scattering experiments, A. Grueneis, D. Vyalikh, A. Bosak, J. Serrano, C. Attaccalite, L. Wirtz, M. Lazzeri, F. Mauri, A. Rubio, T. Pichler
164. *10th International Conference on Atomically Controlled Surfaces, Interfaces and Nanostructures, ACSIN 10*  
September 21-25 2009 Granada, Spain.  
ORAL CONTRIBUTION AND CHAIRPERSON  
- Gd-Au nanotemplates: herringbone, trigons and surface alloy, M. Corso, L. Fernández, F. Schiller, M. Verstraete, A. Rubio, T. Greber, J. E. Ortega
165. *3rd Meeting on High Performance Computing in Molecular Simulation*  
October 1st-2nd 2009, Madrid(Spain)  
ORAL CONTRIBUTION  
- A mixed quantum-classical dynamics with the correct equilibrium distribution. J. L. Alonso, X. Andrade, A. Castro, P. Echenique, M. Marques, V. Polo, A. Rubio y D. Zueco
166. 24rd International Winterschool on Electronic Properties of Novel Materials (IWEPNM2010), March 7-13 (2010), Kirchberg/Tirol, Austria  
POSTERS  
- Computational design of chemical nanosensors: Metal doped carbon nanotubes, D. J. Mowbray, J. M. García-Lastra, K. S. Thygesen, A. Rubio, and K. W. Jacobsen  
- Optical Properties and Electronic Structure of (6,5) enriched SWCNT, K. De Blauwe, C. Kramberger, P. Ayala, F. Simon, Y. Miyata, H. Shiozawa, D.J. Mowbray, A. Rubio, P. Hoffmann, H. Kuzmany, H. Kataura, T. Pichler

167. *Theoretical Spectroscopy: density functional theory and beyond for real materials* Symposium DPG Spring Meeting  
Regensburg March 24 - 26, 2010  
ORAL CONTRIBUTION  
- Bridging rare-earth physics and chemistry: a hybrid functional study for Ce M. Casadei, X. Ren, A. Rubio, and M. Scheffler  
- Evolution of electron traps at ice surface: aggregation of orientational defects, M. Bockstedte, A. Michl and A. Rubio  
- Is there a physical meaning of the natural orbitals? Analysis of exactly solvable models, N. Helbig, J. Fuks, I. Tokatly and A. Rubio
168. *Nanoscale Devices for Environmental and Energy Applications*  
Encuentro Consolider (NDEEA10) 26-27 April 2010 San Sebastián  
ORAL CONTRIBUTION and POSTER  
- Ab-initio optical properties of dyes for hybrid solar cells, a TDDFT approach, U. De Giovannini, L. Chiodo, and A. Rubio  
- Influence of the supramolecular environment in molecular layers on their electronic properties, D.G. de Oteyza, J.M. García-Lastra, M. Corso, B.P. Doyle, L. Floreano, A. Morgante, Y. Wakayama, A. Rubio, J.E. Ortega  
- Computational Design of Chemical Nanosensors: Metal Doped Carbon Nanotubes, D. Mowbray, K. Thygesen, A. Rubio, K. Jacobsen, J.M. García-Lastra
169. *Young Researchers' Meeting 2010: Dedicated to bringing together spectroscopy and quantum transport*  
Jyväskylä, Finland 31-May-4-June (2010)  
ORAL CONTRIBUTION  
- Vibrational Excitation of Molecules in STM-IETS - A Theoretical Approach, J. Walkenhorst, A. Castro, L. Stella, A. Rubio  
- Calculation of the optical properties of solids with meta-GGAs, F. Berardi, X. Andrade, M.A.L. Marques and A. Rubio  
- Assessing Self-Consistency in the GW approach, F. Caruso, X. Ren, P. Rinke, A. Rubio and M. Scheffler  
- Bridging rare-earth physics and chemistry: a hybrid functional study for Ce, M. Casadei, X. Ren, P. Rinke, A. Rubio and M. Scheffler  
- The full dielectric response from time-dependent density functional theory A. Sakko, A. Rubio, M. Hakala, and K. Hämäläinen  
- Excited state properties of TiO<sub>2</sub> bulk versus nanostructures, A. Iacomino, J.M. Garcia-Lastra, L. Chiodo, S. Ossicini, H. Petek and A. Rubio
170.  $\Psi_k$  Conference 2010  
12-16 September 2010, Berlin  
INVITED TALK; CHAIRPERSON, POSTER  
- Excited-state properties of confined water permeating through nanochannels, Y. Pouillon and A. Rubio  
- Time-dependent density functional theory calculations beyond dipole selection rule, A. Sakko, M.O. Jahala, A. Rubio and K. Hamalainen  
- Many body effects in the excitation spectrum of a defect in SiC, M. Bockstedte, A. Marini, O. Pankratov and A. Rubio  
- Theoretical investigation of local vibrational excitations by STM-IETS in molecules, J. Walkenhorst, A. Castro, M. Wanko and A. Rubio  
- Nonlinear response in Density Functional Theory: LDA versus exact, N. Helbig, J. Fuks, M. Casula, M.A.L. Marques, I. Tokatly and A. Rubio  
- Designing multifunctional chemical sensors using metal doped carbon nanotubes, D. J. Mowbray, J. M. Garcia-Lastra, K. S. Thygesen, A. Rubio, and K. W. Jacobsen  
- Applying hybrid functional and many body methods to rare earth: a study of Cerium clusters, M. Casadei, X. Ren, P. Rinke, A. Rubio and M. Scheffler  
- Metal-insulator transition of one-dimension hydrogen chain: a variational Monte Carlo study, L. Stella, C. Attaccalitte and A. Rubio  
- NO Chemistry: Interaction with water clusters, J. Finn, F. Baletto and A. Rubio
171. *DPG Spring Meeting*  
Dresden, 13-18 of March 2011  
CONTRIBUTED TALKS  
- Excited States from *GW*: the role of self-consistency, F. Caruso, X. Ren, P. Rinke, A. Rubio and M. Scheffler

- Applying hybrid functional and many body methods to rare earths: a study of Cerium, M. Casadei, X. Ren, J. Paier, P. Rinke, A. Rubio and M. Scheffler
172. *25th International Winterschool on Electronic Properties of Novel Materials (IWEPNM2011)*, 26-February 5-March (2011), Kirchberg/Tirol, Austria  
POSTERS  
- Using theoretical spectroscopy to assess the measured electronic structure of doped SWCNTs, D. Mowbray, P. Ayala, A. Rubio and T. Pihler
173. *Symposium on Surface Science-2011*, 6-12 March 2011, Baqueira, Spain  
CONTRIBUTED TALK  
- Tailoring interactions in supramolecular networks by fluorination, E. Goiria, A. El-Sayed, D. G. de Oteyzad, M. Matena, C. Rogero, J. M. García-Lastra, D. J. Mowbray, A. Rubio, Y. Wakayama, and J. E. Ortega
174. *March 2011 American Physical Society Meeting*  
Dallas, Texas, USA, 21-25 March 2011.  
INVITED AND CONTRIBUTED TALKS  
- Laser-Shot-Induced Chemical Reactions inside Nanotubes: a TDDFT investigation , H. Zhang, Y. Miyamoto, and Angel Rubio  
- Tuning the Kohn Anomaly in the Phonon Dispersion of Graphene by Interaction with the Substrate and by Doping, Ludger Wirtz, Adrien Allard, Claudio Attaccalite, Michele Lazzeri, Francesco Mauri and Angel Rubio  
- Shedding Light on Solar Cells with Synchrotron Radiation, Franz Himpsel, Peter Cook, Phillip Johnson, Xiaosong Liu, Wanli Yang, Angel Rubio, Juan-Maria Garcia-Lastra, Enrique Ortega, Celia Rogero, Ruben Gonzales
175. *45th annual meeting of the Finnish Physical Society*, Helsinki, Finland, 29-31 March 2011  
CONTRIBUTED TALK  
- New understanding of the lyman-birge-hopfield band of N<sub>2</sub> A. Sakko, J. A. Bradley, G. T. Seidler, M. Hakala, A. Rubio, G. Cooper, A. P. Hitchcock, K. Schlimmer, K. P. Nagle, and K. Hämäläinen
176. *HPC-NN2011 High-Performance-Computing (HPC) for Nanoscience & Nanotechnology* Bilbao, Spain, 14 April, 2011  
POSTER  
- Designing multifunctional chemical sensors using metal doped carbon nanotubes Duncan J. Mowbray, Juan Maria Garcia Lastra, Kristian S. Thygesen, Angel Rubio, Karsten W. Jacobsen
177. *Young Researchers' Meeting 2011* Naples, Italy, May 16 - May 20, 2011  
INVITED and CONTRIBUTED TALKS  
- Modelling Inelastic Electron Tunnelling with TDDFT - Bugs and Features, J. Walkenhorst, M. Wanko, A. Castro and A. Rubio  
- An unified real-time real-space description of Magneto Optical response in closed-shell molecular systems, L.A. Espinosa-Leal, D. Varsano, R. di Felice and A. Rubio  
- Non-adiabatic contributions to the spectrum of simple molecular models: the case of the one-dimensional dihydrogen cation, Alison Crawford Uranga, Lorenzo Stella, Stefan Kurth, and Angel Rubio  
- Chemical accuracy by throwing random numbers? A brief introduction to Quantum Monte Carlo methods, Lorenzo Stella, Claudio Attaccalite, and Angel Rubio  
- Photo-electron Spectroscopy for finite systems with TDDFT, Umberto De giovannini, and Angel Rubio  
- Computational Approaches for Complex Systems, Marius Wanko and Angel Rubio
178. *Third International Meeting on G-Quadruplexes and G-assembly* , Sorrento, Italy, June 28 - July 1, 2011  
INVITED TALK  
- Dynamics and optics of G4-porphyrin stacks, R. Di Felice, L.A. Espinosa-Leal, D. Varsano, A. Rubio
179. *Frontiers in Interface Science: Theory and Experiment 2011*, Berlin, Germany, 28 June - 1 July, 2011  
POSTER  
- Dynamical detuning of rabi oscillations in adiabatic time-dependent density functional theory J. I Fuks, N. Helbig, I. Tokatly, Angel Rubio
180. *European Conference on Surface Science (ECOSS-28)*, 28th August-2nd September 2011, Wroclaw, Poland  
CONTRIBUTED TALK  
- Transparency of Ag steps to surface electrons, E. Ortega, Z. Abd-el-Fattah, M. Matena, M. Corso, F. Schiller, J. Lobo, A. Mugarza and A. Rubio



181. *Workshop on Strong Correlation from First Principles (SC1p)*, Monastery Seon, Germany, August 30 - September 2, 2011  
 INVITED TALK  
 - Phase transitions within the GW approximation, Matteo Gatti and Angel Rubio  
 - A unified description of ground and excited state properties of finite systems: the self-consistent GW approach, Fabio Caruso, Patrick Rinke, Xinguo Ren, Angel Rubio, and Matthias Scheffler
182. *16th ETSF Workshop on Electronic Excitations* Turin, Italy, 27-30 September 2011  
 CONTRIBUTED TALK  
 - Phase transitions within the GW approximation, Matteo Gatti and Angel Rubio
183. *"Fachbeirat Meeting"* (November 6 - 8, 2011) , Berlin  
 - A unified description of ground and excited state properties of finite systems: the self-consistent GW approach, F. Caruso, P. Rinke, X. Ren, A. Rubio, and M. Scheffler  
 - Unravelling the  $\alpha - \gamma$  phase transition in Ce from the nanoscale to bulk, M. Casadei, X. Ren, P. Rinke, A. Rubio, and M. Scheffler
184. *March 2012 American Physical Society Meeting*  
 February 27-March 2, 2012, Boston, MA, USA  
 INVITED AND CONTRIBUTED TALKS  
 - TDDFT for nonlinear phenomena of light-matter interactions, A. Rubio  
 - Performance of the exact adiabatic density functional to describe Rabi physics J.I. Fuks, N. Helbig, H. Appel, I.V. Tokatly, A. Rubio  
 - Time Evolution of Density Matrices Using BBGKY Hierarchy; Ali Akbari , Javad Hashemi , Risto Nieminen , Robert Van Leeuwen , Angel Rubio  
 - Unified description of ground and excited states of finite systems: the self-consistent GW approach, F. Caruso, P. Rinke, X. Ren, A. Rubio and M. Scheffler
185. *DPG Spring Meeting*  
 Berlin, 25-30 March 2012  
 CONTRIBUTED TALKS  
 - Excited States from *GW*: the role of self-consistency, F. Caruso, X. Ren, P. Rinke, A. Rubio and M. Scheffler  
 - Unraveling the  $\alpha - \gamma$  phase transition in Ce from first principles, M. Casadei, X. Ren, P. Rinke, A. Rubio and M. Scheffler  
 - Quantum coherence controls the charge separation in a prototypical artificial light harvesting system, S. M. Falke, C.A. Rozzi, N. Spallanzani, A. Rubio, E. Molinari, D. Brida, M. Maiuri, G. Cerullo, H. Schramm, J. Christoffers, and C. Lienau  
 - Electron Tunneling - The Influence of Interaction, J. Walkenhrst, N. Helnig, H. Appel, E.K.U. Gross and A. Rubio  
 - Treatment of spin in reduced density-matrix functional theory, N. Helbig, N.N. Lathiotakis, S. Kurth, A. Rubio  
 - First principles study of photoinduced charge separation in an artificial light harvesting complex, Carlo Andrea Rozzi, Sarah Maria Falke, Nicola Spallanzani, Angel Rubio, Elisa Molinari, Daniele Brida, Margherita Maiuri, Giulio Cerullo, Heiko Schramm, Jens Christoffers, and Christoph Lienau  
 - Electronic structure of doped hydrocarbon superconductors, Friedrich Roth, Benjamin Mahns, Matteo Gatti, Pierluigi Cudazzo, Bernd Büchner, Angel Rubio, and Martin Knupfer
186. *CECAM Conference: "Energy from the Sun: Computational Chemists and Physicists Take up the Challenge"*  
 10-14 September, 2012, Chia Laguna resort, Cagliari, Sardinia Italy  
 POSTERS  
 - Electronic and optical properties of defective TiO<sub>2</sub> crystal phases within manybody techniques, A. Iacomino, L. Chiodo and A. Rubio  
 - Excite state properties of TiO<sub>2</sub> surfaces and nanostructures. L. Chiodo, M. Palumbo, G. Giorgi, A.H. Romero and A. Rubio
187. *17th ETSF Workshop on Electronic Excitations* Coimbra, Portugal, 2-5 October 2012  
 COMUNICACION ORAL  
 - Ground-state properties from Many-Body Perturbation Theory: is self-consistent GW good enough? Fabio Caruso, Patrick Rinke, Xinguo Ren, Viktor Atalla, Daniel Rohr, Maria Hellgren, Angel Rubio, and Matthias Scheffler

- Resonant Electron Tunneling - Exact vs. DFT Description, J. Walkenhorst, H. Appel, N. Helbig, A. Rubio
  - Nanoplasmonics response of graphene-like systems by Time-Dependent Density- Functional Theory (TDDFT), F. Berardi, L. Stella, P. Garcia González, C. Andrea Rozzi and A. Rubio
188. *CECAM Workshop "Vibrational coupling: most important, often ignored, and a challenge for ab-initio theory"*, November 6, 2012 to November 9, 2012  
POSTERS
- Towards Regularisation in Quantum Mechanics, Johannes Flick, Heiko Appel, Angel Rubio
  - Towards a full trajectory-based formulation of molecular dynamics, G. Albareda, H. Appel, I. Franco, and A. Rubio
189. *2012 MRS Fall Meeting* November 25-30, Boston, Massachusetts  
COMUNICACION ORAL
- The Nature of Radiative Transitions in TiO<sub>2</sub>-based Nanosheets, M. Palumbo, G. Giorgi, L. Chiodo, A. Rubio, K. Yamashita,
190. *March 2013 American Physical Society Meeting*  
March 18-22, 2013, Baltimore, Maryland, USA  
INVITED AND CONTRIBUTED TALKS
- Simulating Lattice Image of Suspended Graphene Taken by Helium Ion Microcopy, Y. Miyamoto, H. Zhang and A. Rubio
  - Density-Functional Theory Applied to Rare Earth Metals: Approaches Based on the Random-Phase Approximation, M. Casadei, X. Ren, P. Rinke, M. Scheffler and A. Rubio
  - The bond-breaking and bond-making puzzle: many- body perturbation versus density-functional theory, F. Caruso, D. Rohr, M. Hellgren, P. Rinke, X. Ren, A. Rubio and M. Scheffler
191. *DPG Spring Meeting (KM)*  
Regensburg, 10-15 of March 2013  
CONTRIBUTED TALKS
- The role of non-linear second-order coupling Hamiltonians in photoemission and Raman spectroscopy, J. Flick, H. Appel, A. Rubio
  - Linear and non-linear responses in pump-probe spectroscopy, T. Dimitrov, H. Appel and A. Rubio
192. *DPG Spring Meeting (AMOP)*  
Hannover, 18-22 of March 2013  
CONTRIBUTED TALK
- Finite-mass effects beyond the Born-Oppenheimer approximation in the spectroscopy of three-body systems, R. Jestädt, H. Appel, A. Crawford-Uranga, L. Stella, A. Rubio
193. *ICMAT 2013 "7th International Conference on Materials for Advanced Technologies"*  
30 June-5 July 2013, Suntec Singapore  
CONTRIBUTED TALK
- Directly Imaging Chemical Reactions at the Single Molecule Level: Observing Reactant and Product Covalent Bond Structure, Dimas DE OTEYZA, Y. Chen, P. Gorman, A. Riss, S. Wickenburg, Z. Pedramrazi, G. Etkin, H-Z. Tsai, D. Mowbray, A. Rubio, M. Crommie, F. Fisher
194. *"Progress In Electromagnetics Research Symposium" PIERS 2013* 12-15 August, 2013 Stockholm, Sweden  
INVITED TALK
- Performance of Non-local Optics When Applied to Plasmonic Nanostructures L. Stella, P. Zhang, F.J. García Vidal, A. Rubio, P. García-González
195. *Recent Progress in Graphene Research*, Tokyo Institute of Technology 9-13 September 2013  
CONTRIBUTED TALK
- Computational Prediction of Image of Graphene Lattice by Newly Developed Experimental Technique: Helium Ion Microscopy, Y Miyamoto, H. Zhang, A. Rubio
196. *"From Pure to Doped Carbon-Based Nano-Materials: Recent Advances and Applications" (HeteroNanoCarb 2013)* Castelldefels (Barcelona) Spain, September 22-28 (2013)  
CONTRIBUTED TALKS
- Optical Spectra and Excitonic Effects in Hetero-Stacked Layers of Transition Metal Dichalcogenides, A. Iacomino, P. Cudazzo, A. Rubio

- On the electronic structure of silicene on Ag(111): strong hybridization effects S. Cahangirov and A. Rubio
  - First principles study of the collective excitations in 2D materials, P. Cudazzo, I. Tokatly and A. Rubio
197. *Workshop: "Learning from the past, looking to the future" from July 2-5, 2013 in Berlin, Germany* CONTRIBUTED TALKS
- Local effective potentials with correct asymptotic behavior in DFT and Reduced-Density-Matrix-Functional Theory, N. N. Lathiotakis, N. Gidopoulos, N. Helbig, A. Rubio
  - Intra-System derivative discontinuities in static DFT and correlated photon-electron wavefunctions in cavity QED, Heiko Appel, Johannes Flick, Tanja Dimitrov, and Angel Rubio
  - The exact Hohenberg-Kohn functional for a lattice model, T. Dimitrov, H. Appel, and A. Rubio
  - Real-time propagations for correlated systems in Fock space J. Flick, H. Appel and A. Rubio
  - Time evolution of reduced density matrices using BBGKY hierarchy Introduction, M.J. Hashemi, A. Akbari, A. Rubio, R. Nieminen and R. van Leeuwen
198. *6th Time-Dependent Density Functional Theory: Prospects and Applications*, 4 - 18 January 2014 Benasque, Spain.
- INVITED TALKS + POSTERS
- Time-dependent density functional theory of magneto-optical response of periodic insulators, I. V. Lebedeva, I. V. Tokatly and A. Rubio (Poster)
  - Non-Adiabatic Dynamics with Conditional Wave Functions. Guillermo Albareda, Heiko Appel, Ignacio Franco, Ali Abedi and Angel Rubio. (talk)
  - Thermoelectrics of the Atomic-Thin Germanene. Kaike Yang, Roberto D'gosta and Angel Rubio (Poster)
  - Real-time evolution of Maxwell systems in spinor representation. René Jestädt, Heiko Appel and Angel Rubio (Poster)
199. *17th Meeting of the Fachbeirat of the FHI workshop. Berlin, 12th - 14th February 2014.* POSTERS
- Unravelling the alpha-gamma Phase Transition in Cerium from the Nanoscale to the Bulk. Marco Casadei, Xinguo Ren, Patrick Rinke, Angel Rubio, and Matthias Scheffler
  - The exact Hohenberg-Kohn functional for a lattice system. Tanja Dimitrov, Heiko Appel, and Angel Rubio.
  - Correlated light-matter interaction in cavity quantum electrodynamics. Johannes Flick, Heiko Appel, and Angel Rubio
  - Real-time propagation of coupled Maxwell-Schrödinger systems. René Jestädt, Heiko Appel, and Angel Rubio.
200. *March 2014 American Physical Society Meeting*  
Denver, Colorado, USA, 3-7 Marzo 2014.
- CONTRIBUTED TALKS
- Energy Level Alignment for Many-Body Resonant Tunneling, J. Walkenhorst, N. Helbig, H. Appel, A. Rubio
  - Time-dependent density functional theory of magneto-optical response of periodic insulators, I.V. Lebedeva, I.V. Tokatly, A. Rubio
  - Identifying individual chemical bonds in single-molecule chemical reaction products using nc-AFM, S. Wickenburg, D. G. de Oteyza, P. Gorman, Y-C. Chen, A. Riss, D.J. Mowbray, G. Etkin, Z. Pedramrazi, Hsin-Zon Tsai, A. Rubio, M. F. Crommie, F. R. Fischer
  - Two-level tunneling systems in amorphous alumina, I.V. Lebedeva, A. Perez-Paz, I.V. Tokatly, A. Rubio
201. *78th Annual Meeting of the DPG and DPG Spring Meeting (AMOP Section)* Berlin, 17 - 21 of March 2014
- CONTRIBUTED TALK
- Non-Adiabatic Molecular Dynamics with Conditional Wave Functions. Guillermo Albareda, Heiko Appel, Ignacio Franco, Ali Abedi and Angel Rubio
202. *DPG Spring Meeting*  
Dresden, 30- March, 4-April 2014
- CONTRIBUTED TALKS
- Is Cerium Unique? Rare Earth Metals in Density-Functional Theory, M. Casadei, X. Ren, P. Rinke, A. Rubio and M. Scheffler
  - Correlated light-matter interactions in cavity QED, J. Flick, H. Appel, A. Rubio
  - The exact Hohenberg-Kohn functional for a lattice model, T. Dimitrov, H. Appel, A. Rubio
  - Real-time propagation of coupled Maxwell-Schrödinger systems, R. Jestädt, H. Appel, A. Rubio

- Optimized effective potential approach to time-dependent density functional theory for many-electron systems inter- acting with cavity photons, C. Pellegrini, J. Flick, H. Appel, I.V. Tokatly, A. Rubio
  - Two-level tunneling systems in amorphous alumina, A. P. Paz, I.V. Lebedeva, I. V. Tokatly and A. Rubio
  - Time-dependent density functional theory of magneto-optical response of periodic insulators, I.V. Lebedeva, I.V. Tokatly and A. Rubio
203. *2014 MRS Spring Meeting* April 21-25, San Francisco, California, Symposium on "Materials and Processes for Nonlinear Optics"  
COMUNICACION ORAL
- Non-linear optical susceptibility and local-field factors in liquid chloroform: A time-dependent density-functional theory study, D.A. Strubbe,, A. Perez-Paz, X. Andrade, A. Rubio, S.G.Louie
204. *E-MRS Spring Meeting 2014 Symposium on Computational Modelling of Organic Semiconductors* Congress Center in Lille (France) from May 26 to 30, 2014.  
COMUNICACION ORAL
- Ultrafast charge generation in a photoexcited polymer-fullerene blend: insights from real-time TDDFT, by Authors : C.A. Rozzi, M. Amato, A. Rubio, and E. Molinari
205. *International Conference on Mathematical Modeling in Physical Sciences. August 28-31, 2014. Madrid, Spain.*  
COMUNICACION ORAL
- Prediction of new 2D materials: after graphene and silicene, now a hint of germanene synthesis, M.E.Davila, L.Xian, S. Cahangirov, A.Rubio and G. Le Lay
206. *Quantum Disordered Systems: What's next? 24-27 June 2014 Toulouse, France.*  
POSTER
- Two-level tunneling systems in amorphous alumina, A. P. Paz, I.V. Lebedeva, I.V. Tokatly and A. Rubio
207. *3M-NANA:O 4th International Conference on Manipulation, Manufacturing and Measurement on the Nanoscale; 27-31 October 2014 Taipei, Taiwan.*  
INVITED TALK
- Silicene Phases on Ag(111), G. Le Lay, S. Cahangirov, L. Xian, A. Rubio
208. *Emerging Non-Graphene 2D Atomic Layers and van der Waals Solids.Symposium of the Fall Materials Research Society (MRS) meeting, Boston (November 30-December 5, 2014)*  
COMUNICACION ORAL and SESSION CHAIR
- A TDDFT-based study on the proton-DNA interaction, M.A.Bernal, G.Brunetto, R.Seraide, U. de Giovannini and A.Rubio
209. *2nd International Symposium on Computics: Quantum Simulation and Design ISC-QSD2014* , 1-5 December (2014), Koshiba Hall in The University of Tokyo, Japan COMUNICACION ORAL
- Photo-enhancement of cohesion: cases of noble atoms and layered amteriasl, Y. Miyamoto, H. Zhang, T. Miyazaki, A. Rubio
210. *Banff Meeting on Structural Dynamics in Canada (15-18. Feb 2015).*  
COMUNICACION ORAL
- Laser induced electron diffraction in aligned molecules. F. Krecinic, F. Braue, A. Rouzee, U. De Giovannini, Q. Zheng, A. Rubio, M. Vrakking
211. *APS March Meeting 2015. San Antonio (Texas) 2-6 March 2015*  
COMUNICACION ORAL
- Correlated Light-Matter Interactions in Cavity QED. J.Flick, H. Appel and A.Rubio
  - Density matrix perturbation theory for magneto-optical response of periodic insulators. I.V. Lebedeva, I.V. Tokatly and A.Rubio
212. *ICMAT 2015 "7th International Conference on Materials for Advanced Technologies"*  
30 June-5 July 2015, Suntec Singapore  
CONTRIBUTED TALK
- Engineering Photophenomena in Self-assembled 3d Van Der Waals Heterostructures M Bala Murali Krishna, Michael Man, Soumya VinoD, Catherine Chin, Takaaki Harada, Jaime Taha-Tijerina, Chandra Sekhar Tiwary, Patrick Nguyen, Patricia Chang, Angel Rubio, Pulickel Ajayan, S aikat Talapatra, Keshav Dani

213.  *$\Psi_k$  Conference 2015*  
 6-10 September 2015, Berlin  
 INVITED TALK; CHAIRPERSON, POSTER  
 -Exact Maps in Density Functional Theory for a Lattice model. T. Dimitrov, H. Appel and A. Rubio  
 - Kohn-Sham Approach to Cavity QED: Exact vs. Approximate Effective Fields. J.Flick, C.Pellegrini, M. Ruggenthaler, H. Appel, I.V.Tokatly and A. Rubio  
 - Time-Evolution of Tensor Networks in Quantum Electro-dynamics. T. Reinhard, H. Appel and A. Rubio  
 - Wave- packet dynamics in lattice quantum electrodynamics.U. Mordovina, H.Appel and A.Rubio  
 - Real-time propagation of coupled Maxwell-Kohn-Sham systems. R. Jestaedt,H.Appel, A.Rubio  
 The atomic and electronic structure of silicene and germanene on substrates S. Cahangirov, L. Xian, A. Rubio  
 - The NoMaD Laboratory and Big-Data Analytics: Extracting hidden information from repositories of computational materials science, F. Mohamed, L. M. Ghiringhelli, C. Carbogno, C. Draxl, A. De Vita, D. Frenkel, F. Illas, R. Nieminen, A. Rubio, K. S. Thygesen, and M. Scheffler  
 -Untangling Excitation Energy Transfer for the LHC-II complex from Full First-Principles Calculations. (Contributed talk) Joaquim Jornet-Somoza, Joseba Alberdi-Rodríguez, Bruce Milne, Xavier Andrade, Miguel A. L. Marques, Fernando Nogueira, Micael J. T. Oliveira, Angel Rubio.  
 -Time-dependent density functional theory of magneto-optical response of periodic insulators. I.V. Lebedeva, I.V. Tokatly and A.Rubio  
 -Optimized Effective Potential for Quantum Electrodynamical Time-Dependent Density Functional Theory. C. Pellegrini, J.Flick, I.V. Tokatly, H. Appel and A. Rubio -Krieger-Li-Iafrate approximation to the optimized effective potential approach in density functional theory for quantum electrodynamics. C. Schäfer, J. Flick, H. Appel, C.Pellegrini and A.Rubio  
 -Optimal thermoelectric figure of merit of SiGe core-shell nanowires. K.Yang, A.Cantarero, A. Rubio and Roberto D'Agosta  
 -Adiabatic and nonadiabatic molecular dynamics with conditional wave functions.G. Albareda,A. Abedi, J. M. Bofilla, I.Tavernellie and A. Rubio -Pilot Applications of the SCE Functional for the Description of Strong Correlation in Adiabatic TDDFT. Mirtschink, U. De Giovannini, A. Rubio and P. Gori-Giorgi
214. *March 2016 American Physical Society Meeting*  
 March 14-18, 2016, Baltimore, Maryland, USA  
 INVITED AND CONTRIBUTED TALKS
- Optical control of inter-layer distance of hBN: a TDDFT study, Yoshiyuki Miyamoto, Hong Zhang, Takehide Miyazaki, and Angel Rubio
  - Stable Dirac semi-metal in the allotrope of IV elements, P. Tang, W.Cao, W. Duan, A. Rubio
215. *The 50th Fullerenes-Nanotubes-Graphene General Symposium*  
 The University of Tokyo, Ito International Research Center, Ito Hall, February 20-22, 2016  
 CONTRIBUTED TALK  
 - Enhancement of laser-induced water decomposition by 2D sheets studied by first-principles simulations, Y. Miyamoto, H. Zhang, X. Cheng, A. Rubio
216. *NT16.17th International Conference on the Science and Application of Nanotubes and low-dimensional materials.* University of Vienna, Austria.7-13 August 2016  
 INVITED TALK  
 - Theory for UV to THZ light conversion using graphene nano-ribbons Yoshiyuki Miyamoto, Hong Zhang, Xinlu Cheng, and Angel Rubio
217. *Fullerenes-Nanotubes-Graphene General Meeting*  
 Sapporo , Hokkaido Island, Japan, 2016  
 CONTRIBUTED TALK  
 - Enhancement of laser-induced water decomposition by 2D sheets studied by first-principles simulations II, Y. Miyamoto, H. Zhang, X. Cheng, A. Rubio
218. *Pacific Rim Symposium on Surfaces, Coatings and Interfaces (PacSurf 2016)*  
 Hawaii December 11 - 15, 2016. INVITED TALK  
 - 1D structures at Stepped Si Surfaces and in Organic Molecules, F. Himpsel, J.M. García Lastra, A. Rubio, I. Boukahil, R. Qiao, S.C. Erwin, I. Barke

219. *APS March Meeting 2017. New Orleans 13-17 March 2017*  
 COMUNICACION ORAL  
 - Charge and energy transport at the nanoscale: A DFT perspective, F. G. Eich , F. Covito , A. Rubio  
 Plasmons in quasi-two-dimensional metals
220. *DPG-Frühjahrstagung (Spring Meeting) of the Condensed Matter Section. Dresden, 19 - 24 March 2017*  
 COMUNICACION ORAL  
 -On the hunt for better functionals in DFT: a new quantum embedding scheme .U. Mordovina, T.E. Reinhard, H.Appel and A.Rubio  
 -Impact of the electronic band structure in high-harmonic generation spectra of solids.N. Tancogne-Dejean,O. D. Mucke, F.X. Kartner and Angel Rubio  
 Contribution submission to the conference Dresden 2017 -Charge and energy transport at the nanoscale: A DFT perspective, Florian G. Eich, Fabio Covito, and Angel Rubio  
 - Ab-Initio Description of Photoinduced Processes Beyond Classical Maxwell Theory — N. Hoffmann, C. Schaefer, H. Appel and A. Rubio  
 - Density matrix embedding theory for coupled fermion-boson systems — T. E. Reinhard, U. Mordovina, H. Appel, J. S. Kretchmer, G. K. L. Chan, and A. Rubio  
 - Intercalated porphines at the BN/Cu(111) interface: structure, electronic properties and function — J. Dücke, A. Riss, A. Pérez Paz, A. Rubio, J. V. Barth, and W. Auwärter  
 -Accessing micro- and mesoscopic ultrafast electron dynamics in low-dimensional materials — M. Puppini, C. Nicholson, M. Müller, R. Bertoni, H. Hübener, A. Rubio, C. Monney, C. Cacho, M. Wolf, A. Paarmann, L. Rettig, and R. Ernstorfer
221. *DPG Frühjahrstagung (Spring Meeting) of the Atomic, Molecular, Plasma Physics and Quantum Optics Section (SAMOP). Mainz, 6 - 10 March 2017*  
 COMUNICACION ORAL  
 - Cavity-QED beyond model systems.C.Schaefer,J. Flick, H.Appel, C. Pellegrini and A.Rubio - Ab-Initio Description of Photoinduced Processes Beyond Classical Maxwell Theory.N. Hoffmann, H. Appel and Angel Rubio
222. *CLEO: Conference on Lasers and Electro-Optics and the European Quantum Electronics Conference, 14-19 May 2017, San Jose, California*  
 INVITED  
 - *Ellipticity dependence of higher-order harmonics in solids: unraveling the coupled intraband and interband dynamics*, N. Klemke, G. Di Sciacca, Y. Yang, G. M. Rossi, R. E. Mainz, N. Tancogne-Dejean, A. Rubio, F. X. Kärtner, and O. D. Mücke
223. *CLEO EU: The European Conference on Lasers and Electro-Optics and the European Quantum Electronics Conference, 25-29 June 2017, Munich Germany*  
 INVITED  
 - *Ellipticity dependence of higher-order harmonics in solids: unraveling the interplay between intraband and interband dynamics*, N. Klemke, G. Di Sciacca, Y. Yang, G. M. Rossi, R. E. Mainz, N. Tancogne-Dejean, A. Rubio, F. X. Kärtner, and O. D. Mücke
224. *6th International Conference on Attosecond Physics, 2-7 July 2017, Xi'an, China*  
 INVITED  
 - *Circularly polarized high-order harmonics from solids driven by single-color infrared pulses*, N. Klemke, G. Di Sciacca, Y. Yang, G. M. Rossi, R. E. Mainz, N. Tancogne-Dejean, A. Rubio, F. X. Kärtner, and O. D. Mücke
225. *XXXVI Reunión Bienal de la Real Sociedad Española de Física , 17-21 July, 2017, Santiago de Compostela, Spain*  
 CONTRIBUTED TALK and POSTER  
 - *Time-dependent density functional theory of magneto-optical response of solids*, I. V. Lebedeva, I. V. Tokatly, A. Rubio
226. *The 53rd Fullerenes-Nanotubes-Graphene General Symposium. Kyoto University. Uji Campus.Kyoto September 13-15, 2017*  
 CONTRIBUTED TALK  
 -*Carbon Nanotube as a Laser-Field Amplifier for Efficient Water Decomposition: A TDDFT Study*Y. Miyamoto, H. Zhang, X. Cheng and A. Rubio

227. *APS March Meeting, 2018.5-9 March 2018. Los Angeles Convention Center (USA)*  
 - Phonon-driven spin dynamics in the valleys of TMDC. Dongbin Shin, Hannes Hübener, Umberto De Giovannini, Hosub Jin, Angel Rubio and Noejung Park  
 - Laser-induced water decomposition near 2D sheets studied by TDDFT, Y. Miyamoto, H. Zhang, X. Cheng, A. Rubio  
 - Correlated Electron-Photon Excitations within Quantum Electrodynamical Density-functional Theory, J. Flick, D. Welakuh, M. Ruggenthaler, H. Appel, A. Rubio  
 - Light-matter interaction in the long-wavelength limit: necessity of the dipole self-energy, V. Rokaž, D. Welakuh, M. Ruggenthaler, A. Rubio  
 - The Auger process from time dependent density matrix evolution in the GKBA, F. Covito, E. Perfetto, A. Rubio and G. Stefanucci  
 - Light-Matter Interactions via the Exact Factorization Approach, N. M. Hoffmann, H. Appel, A. Rubio, N. T. Maitra
228. *DPG-Frühjahrstagung (Spring Meeting) of the Condensed Matter Section. Berlin, 11 - 16 March 2018*  
 COMUNICACION ORAL  
 -Reduced Density Matrix Theory for Coupled Fermion-Boson Systems. F. Buchholz, I. Theophilou, M. Ruggenthaler, H. Appel and A. Rubio  
 -Selfconsistent density embedding - a new class of functionals for DFT. Uliana Mordovina, Teresa E. Reinhard, Heiko Appel and Angel Rubio  
 -Phase transition of the 2D Hubbard-Holstein model. Teresa E. Reinhard, Uliana Mordovina, Heiko Appel and Angel Rubio  
 -Coupling Maxwell's equations to the time-dependent Kohn-Sham equations: near-field effects and electromagnetic backreaction. R. Jestädt, M. Oliveira, A. Rubio, H. Appel  
 -Transient charge and energy flow in the wide-band limit, F. Covito, F. Eich, R. M. Sentef, A. Rubio  
 -Dissipative exchange-correlation functional in QED-TDDFT. Camilla Pellegrini, Ilya Tokatly and Angel Rubio  
 - Reduced Density Matrix Theory for Coupled Fermion-Boson Systems, F. Buchholz, I. Theophilou, M. Ruggenthaler, H. Appel, A. Rubio
229. *Strong Coupling with Organic Molecules (SCOM 2018), Eindhoven, April 16-18 (2018) POSTERS*  
 - Enhancing excitation energy and charge transfer with strongly correlated light-matter interaction, C. Schafer, et al  
 - Density-functional reformulation of matter-photon problems, M. Ruggenthaler et al  
 -Correlated Electron-Photon Excitations within Quantum Electrodynamical Density-functional Theory, D. Welakuh et al  
 - Light-matter interaction in the long-wavelength limit: necessity of the dipole self-energy, V. Rokaž et al
230. *CLEO 2018: Conference on Lasers and Electro-Optics*, 13-18 May 2018, San Jose, California  
 INVITED  
 - High-Order Harmonic Generation from Solids Dressed by an Intense Terahertz Field, H. Huang; L. Song; N. Tancogne-Dejean; N. Klemke; A. Rubio; F. Kaertner; O. Muecke  
 - Strong-Field Polarization-State Control of Higher Harmonics Generated in Crystalline Solids, N. Klemke; N. Tancogne-Dejean; G. Rossi; Y. Yang; R. Mainz; G. Di Sciacca; E. Casandruc; A. Rubio; F. Kaertner; O. Muecke
231. *XXI International Conference on Ultrafast Phenomena. Hamburg (Germany)-15-20 July 2018*  
 -Polarization states of high-harmonics generated in silicon from elliptical drivers. N. Klemke, N. Tancogne-Dejean, G. M. Rossi, Y. Yang, R. E. Mainz, G. Di Sciacca, A. Rubio, F. X. Kartner and O. D. Mücke  
 -Strong-field physics in the molecular frame. Andrea Trabatttoni, Sebastian Trippel, Umberto De Giovannini, Jean Francois Olivieri, Joss Wiese, Terry Mullins, Jolijn Onvlee, Sang-Kil Son, Biagio Frusteri, Angel Rubio and Jochen Kopper  
 -NIR-assisted stabilization of adenine following ionization by XUV attosecond pulses. E. P. Månsson, M. Gall, V. Wanie, S. Latini, U. De Giovannini, M. C. Castrovilli, F. Frassetto, L. Poletto, J. Greenwood, F. Légaré, M. Nisoli, A. Rubio and F. Calegari
232. *IRMMW-THz conference, 9-14 September, Japan*  
 CONTRIBUTED TALK  
 - Ultrafast Control of Even-Order Harmonic Generation from Solids by an Intense Terahertz Field, H. Huang, L. Song, N. Tancogne-Dejean, N. Klemke, A. Rubio, F. X. Kärtner, O. D. Mücke

233. APS March Meeting, 2019.4-8 March 2019. Boston Convention and Exhibition Center (BCEC)  
 CONTRIBUTED TALKS  
 -Cavity-enhanced electron-phonon coupling in monolayer FeSe/SrTiO<sub>3</sub>r, M. Sentef, M. Ruggenthalert, A. Rubio  
 -Orbital magneto-optical response of periodic insulators from first principles. D. Strubbe, I. V. Lebedeva, I. V. Tokatly, A. Rubio  
 -Floquet behavior of correlated systems with light-matter coupling. N. Kalthoff
234. *CLEO 2019: Conference on Lasers and Electro-Optics*, 5-10 May 2019, San Jose, California  
 CONTRIBUTED TALK  
 -Time-domain vectorial field reconstruction of a circularly polarized harmonic from silicon using 2D spectral shearing interferometry. F. Scheiba, N. Klemke, N. Tancogne-Dejean, G. M. Rossi, A. Rubio, O. D. Mücke and F. X. Kärtner
235. *CLEO/Europe-EQEC 2019*, 23 – 27 June 2019, Munich, Germany CONTRIBUTED TALKS  
 -Attosecond electron localization and screening dynamics in metals. M. Volkov, S. Sato, F. Schlaepfer, L. Kasmi, N. Hartmann, Gallman, A. Rubio and U. Kelleri  
 -Optically driven attosecond electron dynamics in gallium arsenide. F. Schlaepfer, M. Lucchini, S. A. Sato, M. Volkov, L. Kasmi, Keller
236. *7th International Conference on Attosecond Science and Technology (ATTO2019)* Szeged, Hungary from July 1 to 5 2019,  
 CONTRIBUTED TALK  
 - Polarization-state-resolved high-harmonic spectroscopy of solids, N. Klemke, N. Tancogne-Dejean, G. M. Rossi, Y. Yang, F. Scheiba, R. E. Mainz, G. Di Sciacca, A. Rubio, F. X. Kärtner, O. D. Mücke
237. *QUTIF Annual Meeting 26-28 February 2020 in Berlin*  
 CONTRIBUTED TALK  
 -Circularly polarized high harmonics from solids originating from intraband dynamics. N. Klemke, N. Tancogne-Dejean, A. Rubio, F. X. Kärtner and O. D. Mücke
238. *APS March Meeting, 2020, 2-6 March 2020. Denver, Colorado, USA*  
 CONTRIBUTED TALKS  
 -Quantum cavities and Floquet materials engineering from first principles QEDFT. A. Rubio  
 -Ultrafast laser-assisted photoprotection mechanism in the adenine cation. Erik P. Maansson, Simone Latini, Fabio Covito, Vincent Wanie, Mara Galli, Enrico Perfetto, Gianluca Stefanucci, Hannes Hubener, Umberto De Giovannini, Mattea C. Castrovilli, Andrea Trabattoni, Fabio Frassetto, Luca Poletto, Jason B. Greenwood, Francois Legare, Mauro Nisoli, Angel Rubio and Francesca Calegari  
 -Excitonic effects from real-time parameter-free hybrid functions. Nicolas Tancogne-Dejean, Angel Rubio  
 -Time-dependent magnons from first principles. Nicolas Tancogne-Dejean, Florian Eich, Angel Rubio  
 -Observables of real-time lattice dynamics in time-dependent density functional theory. Hannes Huebener  
 -Emergent topological phases in synthetic dimensions with low-frequency laser pumping. Peizhe Tang, Shunsuke Sato, Angel Rubio  
 -Cavity Induced Non-adiabatic Effects and Modifications of the Spin-orbit Coupling. Dominik Urs Sidler  
 -Recent developments in the Octopus code for strong light-matter coupling. Micael Oliveira -Topological Floquet engineering of twisted bilayer graphene. Michael Sentef, Gabriel E. Topp, Gregor Jotzu, James W. McIver, Lede Xian, Angel Rubio  
 -Real space and real time electron dynamics simulations for attosecond physics in solids. Shunsuke Sato  
 -Quantum dynamics in driven spin systems with neural-network quantum states. Damian Hofmann, Giuseppe Carleo, Angel Rubio, Michael Sentef  
 -Mixed Quantum-Classical Methods for Molecules in Cavities. Norah M. Hoffmann, C Schäfer, L. Lacombe, Aaron Kelly, Heiko Appel, Neepa T. Maitra and Angel Rubio  
 -Ab-initio photo-ionization dynamics without continuum states. Umberto De Giovannini  
 -Cavity controlled inverse harmonic generation. Davis Welakuh  
 -Nonadiabatic Electron Nuclear Dynamics in TDDFT with Variational Quantum Nuclei. Kevin Lively, Guillermo Albareda, Aaron Kelly, Shunsuke Sato, Angel Rubio
239. *The 22nd International Conference on Ultrafast Phenomena, July 19-24, 2020. Shanghai. China*  
 CONTRIBUTED TALKS  
 -Attosecond dynamical Frank-Keldysh effect in core excitons. M. Lucchini, S. A. Sato, G. D. Lucarelli, B. Moio, G.



Inzani, R. Borrego-Varillas, F. Frassetto, L. Poletto, H. Huebener, U. De Giovannini, A. Rubio and M. Nisoli - Non-Equilibrium Light-Induced Lifshitz Transition in the Correlated Weyl Semimetal Td-MoTe<sub>2</sub>. S. Beaulieu, S. Dong, N. Tancogne-Dejean, M. Dendzik, T. Pincelli, J. Maklar, R. Patrick Xian, M. Wolf, M. A. Sentef, A. Rubio, L. Rettig and R. Ernstorfer

240. *QUTIF International Conference 22-25 February 2021 (virtual)*

CONTRIBUTED TALK

- Theoretical investigation of high harmonics generation from liquid water, Zahra Nourbakhsh, Ofer Neufeld, Nicolas Tancogne-Dejean, Angel Rubio
- Ab-initio cluster approach for high harmonic generation in three-dimensional liquids: characteristic features, Ofer Neufeld, Zahra Nourbakhsh, Nicolas Tancogne-Dejean, Angel Rubio

241. *APS March Meeting 2021. March 15-19 Online*

CONTRIBUTED TALK

- Conditional wavefunction approach to the structure and dynamics of quantum systems. Guillermo Albareda, Kevin Lively, Shunsuke Sato, Aaron Kelly, Angel Rubio
- Vibronic Spectra from First Principles: Capturing the Franck-Condon Effect without Born-Oppenheimer Surfaces. Kevin Lively, Aaron Kelly, Shunsuke Sato, Guillermo Albareda, Angel Rubio
- Light-induced topological phases in 2D materials. Angel Rubio (Invited talk)
- Light induced topological phases in two-dimensional van der Waals heterostructures. Angel Rubio

**X. PARTICIPACIÓN EN COMITÉS INTERNACIONALES. PUESTOS DE RESPONSABILIDAD**

- *Scientific Advisory Board for the 28th General conference (CMD28) and 29th General conference (CMD29)* of the Condensed Matter Division (CMD) of the European Physical Society (EPS), 31 August-4 September 2020 (Madrid) and 22-28 August 2021 (Manchester)
- *External Review Committee of The Center for Computational Sciences (CCS)*, University of Tsukuba (17-21 February 2020)
- Member of the Scientific advisory board (SAB) of the research field "Information" at the Karlsruhe Institute of Technology (KIT)(2019-2023)
- Full Professor, University of Hamburg, Hamburg (since June 2016-)
- Member of the Scientific Advisory Board of the "Fundacion GADEA por la Ciencia", Spain (2017-)
- Member of the External Scientific Advisory Board of CIQUIS ("Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares") Universidad de Santiago de Compostela (USC) (2017-)
- Member of the Scientific advisory board (SAB) of the C2SEPTEM computational center funded by the U.S. Department of Energy, Office of Science, Berkeley USA (2017-)
- Scientific Academic Advisory Committee (SAAC) review of the area of Organic Chemistry and Material Science (2018) at the Weizmann Institute of Science in Israel (2018)
- Miembro del "Alto Consejo Consultivo en I+D+I de la Generalitat Valenciana" (2015-)
- Member of the Scientific Advisory Committee of CECAM (since 2015-)
- Faculty member of the Wolfgang Pauli Centre, Hamburg (2015-)
- Member of the Scientific Council of ZCAM ("Zaragoza Scientific Center for Advance Modeling") (2013-)
- Member of the "Centro de excelencia en Nanociencia Molecular ISIC-NANO", Valencia (2012-)
- Member of the Scientific advisory board (SAB) of MICCoM (Midwest Integrated Center for Computational Materials), a DOE Computational Materials Science (CMS) Center at Argonne, Chicago, U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences (2016-2019)
- Member of the Science and Software advisory board (SSAB) Molecular Sciences Software Institute (MolSSI) (molssi.org) funded by the National Science Foundation (2017-2019)
- Chair of the European Theoretical Spectroscopy Facility (ETSF) (<http://www.etsf.eu>) (since 2012-2014); Vice-President for Scientific Development (since 2008-2014) and member of the Steering Committee.
- Host group for the HPC++ Europe (Barcelona Supercomputing Center) (<http://www.hpc-europa.org>)
- Member of the BIFI "Instituto de Biocomputación y física de sistemas complejos", Zaragoza, Spain (since January 2008-)
- Member of the "Comissão Externa Permanente de Aconselhamento Científico -CEPAC" (Permanent External Commission for Scientific Advising) of the "Centro de Física Computacional-CFC" (Centre for Computational Physics, Coimbra Portugal (since 2010-)
- Member of the Scientific Council of the GDR-E Nano-I on Science and Applications of Nanotubes, CNRS (France) (2007-); (CSIC-CNRS collaborative agreement)
- Steering Committee and council member of the Marie Curie Series of Events program: Psi-k Training in Computational Nanoscience (<http://www.mc-psi-k-training.cecama.org/>) MSCF-CT-2005-029252 (2006-)
- Member of the Board of Directors (Trustee and foundation member, 15-10-2008) of the Psi-k: UK Charity Commission (Psi-K-1126308): Daresbury Laboratory, Daresbury Science and Innovation Campus, Daresbury, Warrington WA4 4AD Registered in England under company number 06440198 (<http://www.psi-k.org/>).

- External Advisory Board Member of *The center for Nanotechnology and Molecular Materials*, Wake Forest University, North Caroline, USA (Director Prof. D.L. Carroll). (2007-)
- Spanish representative in the Steering Committee of ESF Research Networking Programmes- INTELBIOMAT ("Interdisciplinary Approaches to Functional Electronic and Biological Materials") (June 2008- June 2013)
- UPV/EHU coordinator of the "Doctorate in Materials Science and European Doctorate in Physics and Chemistry of Advanced Materials" <http://www.mater.unimib.it/pcam/> (2005-2008)
- Co-cordinador del Grupo de Trabajo: Nanobiotecnologia de la red NANOSPAIN (<http://www.nanospain.org/>) (2006-2009)
- Advisory Board Member and Physical Scientist associated to the *ITR: Institute for the Theory of Advanced Materials in Information Technology (ITAMIT)*, University of Minnesota, (Director Prof. J. Chelikowsky). Supported by the National Science Foundation (2003-)
- Miembro de la comisión de informática de la Facultad de Ciencias de la Universidad de Valladolid (2000)

## XI. ORGANIZACIÓN Y PARTICIPACIÓN EN ACTIVIDADES DE I+D

- Co-organiser of series of conferences HeteroNanoCarb (2019,2018,2017,2016): international Hetero-Nan”Advances and Applications in Carbon Related Nanomaterials: From pure to doped structures including heteroatom layers”.Benasque (Aragon-Spain).
- Co-organizer of the CECAM-Psik Research Conference ”Ultrafast Physics from molecules to nanostructures”, October 7, 2019 – October 10, 2019, San Sebastian, Spain
- Member of the International advisory Board of the workdop From the NanoWorld to StarDust.NW2SD International conference.Campus du Pharo, Aix-Marseille Université, Jardin du Pharo, 58 Bd Charles Livon, 13007 Marseille.July 17-19 2019, Marseille, France
- Co-organizer of the Flatiron Workshop Quantum Cavities and Excitonic Insulators .8-12 July 2019, CCQ-Flatiron Institute, New York, USA.
- Co-organizer of the Flatiron Workshop.Resonant X-Ray Scattering (RIXS) Workshop.28 February-2 March 2018, CCQ-Flatiron Institute, New York, USA.
- Co-organizer of the Flatiron Workshop.Quantum Chemistry Workshop. November 20-21,2017, CCQ-Flatiron Institute, New York, USA.
- Co-organizer of the Flatiron Workshop.Strong Light-matter Interactions in Chemistry and Materials Science.October 10-12,2017, CCQ-Flatiron Institute, New York, USA.
- Co-organiser of the CECAM-Psik Workshop on Charge carrier dynamics in nanostructures: optoelectronic and photo-stimulated processes, 9th – 13th October 2017, in Bremen, Germany
- Co-organiser of the DPG 2017 Symposium.”Frontiers of Electronic-Structure Theory:New Concepts and Developments in Density Functional Theory and Beyond”.Dresden 19-24 March 2017.
- Scientific Advisor to the workshop ”Frontiers in Physical Sciences” at the International Center for Advanced Studies (ICAS), 16-18 November 2016, Buenos Aires, Argentina
- Advisory Committee for the conference Femto 13: Frontiers of Ultrafast Phenomena in Physics, Chemistry, and Biology, Cancun, Mexico August 13-17, 2017.
- Co-chair of the Workshop on ”Spectroscopy and Dynamics of Photoinduced Electronic Excitations”, ICTP, Trieste 8-12 May 2017.
- Co-chair of the DPG 2017 Symposium.”Frontiers of Electronic-Structure Theory: New Concepts and Developments in Density Functional Theory and Beyond”, Dresden 19-24 March 2017
- Co-director of the series of Schools and workshops on: ”Time-Dependent Density-Functional Theory: Prospects and Applications”, Benasque Center for Science, Benasque, Huesca (Spain) August 29-September 11, (2004); August 26-September 11, (2006); August 31-September 14, (2008); 2-15 January (2010); 4-17 January (2012); 4-18 January (2014); 12-23 September (2016)
- Chair of the workshop on ”Theoretical challenges: simulating materials out of equilibrium”, CFEL, Hamburg, June 1-3, 2016.
- Co-Chair of the Conference ”Advances and Applications in Carbon Related Nanomaterials: From pure to doped structures including heteroatom layers (HNC2015)”, December 7-11, 2015, Benasque (Aragon), Spain
- Chair of the Psi-k-2015 Conference, 6-10 September 2015, San Sebastian-Donostia, Spain
- Member of the committee on ”Optical Interactions with Condensed Matter and Ultrafast Phenomena” at CLEO/QELS 2013 (Conference on Lasers and Electro-Optics), 9-14 June 2013 San Jose Convention Center, San Jose, CA, USA
- Co-chair of the ECI-2013 conference ”From Pure to Doped Carbon-Based Nano-Materials: Recent Advances and Applications (HNC2013)”, September 22-28, 2013 Sitges, Barcelona, Spain

- Co-chairman of the Symposium Multiscale Modeling of Photonic Materials MMM (Multiscale Materials Modeling), Biopolis, Singapore, 15-19 October 2012
- Co-organiser of the "2011 MRS Spring Meeting (Symposium YY: Computational Semiconductor Materials Science)", Moscone West and San Francisco Marriott, San Francisco, California, from April 25 to 29, (2011)
- Member of the International Advisory Board of the European Conference on Molecular Electronics (ECME-2011), September 7-10, 2011, Barcelona (Spain).
- Co-chairman of the "Density functional methods for electronic structure calculations" symposium of the XXII Congress and General Assembly of the International Union of Crystallography, Madrid, Spain, August 22-30, 2011
- Co-organiser of the CECAM workshop on "Challenges and Solutions in GW Calculations for Complex Systems" 7-10 June 2011, CECAM HQ, EPFL, Lausanne, Switzerland
- Co-organiser of the ZCAM workshop "Databases in Quantum Chemistry", Zaragoza 22-24 September 2010.
- Member of the Prize Committee "Psi-k Volker Heine Young Investigator Award", 12-16 September 2010, Berlin, Germany
- International Scientific Committee of the Pan American Advance Study Institute (PASI) on "Electronic Properties of Complex Systems" Cartagena, Colombia. (2010)
- Co-organiser of the CECAM workshop Electronic-structure challenges in materials modeling for energy applications, 1-4 June 2010, CECAM HQ, EPFL, Lausanne, Switzerland
- Scientific Committee of the "International Conference on Advanced Materials Modelling (ICAMM-2010)", Institut des Matériaux Jean Rouxel (IMN), Nantes France 8-10 July 2010, and (ICAMM 2012, 11-16th June 2012).
- Co-organiser of the Symposium "Theoretical Spectroscopy: density functional theory and beyond for real materials" at the Deutsche Physikalische Gesellschaft (DPG) Spring Meeting, Regensburg March 22-26 (2010)
- Scientific Advisory Board of the GDR-E meeting, 19-23 October 2009, Hotel Marvel Coma-Ruga, Salou (Costa Daurada)
- Co-organiser of the CECAM workshop "Computational Challenges emerging from Next Generation Light Sources", 12-15 October 2009, DESY Hamburg, Germany
- International Advisory Board of the Cnano'09 International Conference on Carbon Nanostructured Materials, October 4-8, 2009 Santorini, Greece
- Member of the Scientific Organising Committee of the 10th International Conference on Atomically Controlled Surfaces, Interfaces and Nanostructures, ACSIN 10, September 21-25 2009 Granada, Spain.
- Local Organiser of "Summer School on Simulation Approaches to Problems in Molecular and Cellular Biology", Directors P. Carloni, M. Parrinello. U. Rothlisberger, Palacio Miramar, 31-Agosto, 5 Septiembre 2009, Donostia, Spain.
- Chair of the Gordon Research Conference Time-Dependent Density Functional Theory, New Hampshire, USA, 5-10/07 2009 (Co-chair: M. Marques and vice-chairs Troy Van Voorhis and Fillipp Furche)
- Co-director of the SANES workshop "Integrated Self-Adjusting Nano-Electronic Sensors" San Sebastián, 26-27 February 2009
- Member of the Scientific Committee of the "International Conference on Materials Discovery and Databases: Materials Informatics and DFT", Oran, Algeria, 11-13 October 2008 and "Workshop on Materials Discovery and Databases" November 06 to 08, 2010 at Algiers (Algeria)
- Co-organiser of the "Ab-initio Many Body Theory" (Marie Curie series of events programme: Psi-k Training in Computational Nanoscience); Curso de Verano de la UPV/EHU, Donostia 23-27 Julio (2007)

- Miembro del “Programm Committee” de la conferencia: *International Winterschool on Electronic Properties of Novel Materials Molecular Nanostructures (IWEPNM)* desde el 2003  
Marzo, Kirchberg/Tirol, Austria
- Member of the International Advisory Committee of TNT2005 “Trends in Nanotechnology”,  
Oviedo, 29 Agosto-2 Septiembre 2005  
TNT2007, Donostia, 3-7 September 2007  
TNT2008, Oviedo, 1-5 September 2008  
and TNT2008, Barcelona, 7-11 September 2009.
- Vice-chair of the Gordon conference “Time-Dependent Density-Functional Theory”, Colby College Waterville,  
ME, USA, July 15-20, 2007
- Member of the Scientific Committee of the Third International Workshop on DFT Applied to Metals and Alloys  
(The Materials Genome Project). Oran, Algeria, 2-4 May 2007
- Member of the Scientific Committee of Cargèse International School, Cargèse, Corsica, France 3-15 Julio 2006  
and Member of the Organizing Committee of the NATO ASI School on *Carbon Nanotubes: From Basic Research  
to Nanotechnology* Sozopol, Bulgaria 21-31 May (2005).
- Member of the Programm Committee of the “Nanotechnology II” Symposium (EMT103) of the SPIE’s confer-  
ence on “*Microtechnologies for the New Millenium 2005*”  
Sevilla, Spain 9-11 May 2005
- Co-organiser of the MRS Symposium HH on Functional Carbon Nanotubes, Boston, November 28-December 3  
(2004).
- Member of the Programm Committee of ECOF2004 “European Conference on Organised Films”, responsible  
for the Nanostructures section  
Valladolid, July 22-27 (2004)
- Co-chair of the Symposium “Modelling and Simulationg Materials Nanoworld” of the 3rd International Confer-  
ence “Computational Modelling and Simulation of Materials”  
Acireale (Catania), Sicily, Italy (May 30-June 4 2004).
- Co-organiser of the workshop “*Ab-initio Electron-Excitations Theory: Towards Systems of Biological Interest*”  
and “*Quantum Transport meeting*”  
San Sebastián, September 19-23 2003.
- Co-chair of the “Nanotechnology” Symposium (EMT103) of the SPIE’s conference on “*Microtechnologies for  
the New Millenium 2003*”  
Maspalomas, Gran Canaria, Spain 19-21 Mayo 2003.
- Codirector del Curso de Verano de la UPV/EHU “*Towards atomic scale- and time- resolution at interfaces*”  
San Sebastián/Donostia, 1-5 Julio 2002
- Organizador del Workshop “*Electronic Transport in Nanotubes*” y COMELCAN meeting  
dIPC, San Sebastián/Donostia 3-5 Junio 2002.
- Organizador del *Symposium 49 “Nanostructured Materials”* de la 19<sup>th</sup> General Conference of the Condensed  
Matter Division of the European Physical Society.  
Brighton, UK 7-11 Abril 2002
- Coorganizador del Workshop *Total Energy Methods in Computational Condensed Matter*  
La Laguna, Tenerife, España. 10-12 Enero 2002
- Coorganizador del *2001 NANOPHASE Workshop: “Nanoscale Photon Absorption and Spectroscopy with Elec-  
trons”*  
Centre Europeen de Calcul Atomique et Moleculaire (CECAM), Lyon, France, 12-13 Octubre 2001
- Coorganizador de la conferencia Internacional “*Nanotube 2001 (NT’01)*”, Postdam, Alemania, 22-26 Julio 2001
- Miembro del “International Advisory Commettee” del congreso: “*Electronic Structure: Prediction and Appli-  
cations (ESPA)*”  
San Sebastian, España, 4-6 Octubre 2000.

- Codirector del *CECAM and ESF-PsiK Workshop: "Excited Electronic States and Related Spectroscopic Properties"*  
Centre Europeen de Calcul Atomique et Moleculaire (CECAM), Lyon, Francia, 20-23 Julio 2000.
- Core-group member and Spokesperson of the Nanostructures and nanotechnologies working group of the psi-k network (European Science Foundation Program "Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces" and now "Towards Atomistic Materials Design").  
Miembro del International Advisory Board for the Psi-k 2000 Conference in Schwäbisch Gmünd, Alemania (22-26 Agosto 2000); Psi-k 2005 Conference "Towards Atomistic Materials Design" Schwäbisch Gmünd, Germany, 17-21 September 2005; and Psi-k 2010 Conference , Berlin (12-16 September 2010)
- Codirector del *CECAM and ESF-PsiK Workshop: "Calculation of Electronic Excitations in Finite and Infinite Systems"* Centre Europeen de Calcul Atomique et Moleculaire (CECAM), Lyon, Francia, 1-3 Septiembre 1999.
- Director del *NAMITECH Workshop: "Nanotubes for Microstructure Technology"* Universidad de Valladolid, España. 17-21 Febrero 1997.
- Codirector del *EXCAM Workshop: "Spectroscopy of Electronic Excitations in Materials"*. Universidad de Valladolid, España. 7-9 Septiembre 1998.
- Codirector de la *III Reunión de Materiales Avanzados: Nanotecnologías*. 5-Abril-5-Mayo 1995, E.T.S. Ingenieros Industriales. Valladolid.

## XII. PATENTES Y MODELOS DE UTILIDAD

1. A. Rubio, y J.A. Alonso  
*Nueva fuente de emisión electrónica constituida por nanoestructuras tubulares de nitruro de boro y su fabricación*  
Universidad de Valladolid. Concedida P-9802690 (3-9-2001).
2. A. Rubio y C. Attacalite  
*Gated-controlled light-emitting device made of BN nanotubes with defects* Universidad del País Vasco UPV/EHU (201130228, ID02207561); US-2014-0014900-A1

## XIII. ESTANCIAS EN CENTROS DE INVESTIGACIÓN

**Clave: D= doctorando, P = postdoctoral, I = invitado, C = contratado, O = otras**

1. *Departamento de Física. Universidad de las Islas Baleares*  
Palma de Mallorca, 1-6 de Mayo de 1989.  
Invitado por el Departamento de Física de la UIB. Profesor M. Barranco. I
2. *Fritz-Haber-Institut der Max-Planck-Gesellschaft*  
Berlín, Alemania, 4-Noviembre, 20-Diciembre de 1989. Profesor W. Ekardt  
Tema: "*Propiedades Ópticas de Micropartículas Metálicas*"  
Beca de Movilidad del Personal Investigador de la Universidad de Valladolid. O
3. *Universite de Nancy I*  
Laboratoire de Physique du Solide. Nancy, Francia, 20-Mayo, 15-Junio de 1990.  
Acciones Integradas Hispano-Francesas. Profesor H. Dreyssé O
4. *Fachbereich Physik. Universität Osnabrück*  
Osnabrück, Alemania, Febrero y Marzo de 1991. Profesor G. Borstel  
Tema: "*Propiedades de Clusters Metálicos usando LMTO y TB-LMTO*".  
NATO Collaborative Research Grant y Beca de Movilidad del Personal Investigador de la Universidad de Valladolid. O

5. *Universite de Nancy I*  
Laboratoire de Physique du Solide. Nancy, Francia, Abril de 1991.  
Acciones Integradas Hispano-Francesas. Profesor H. Dreyssé O
6. *Departamento de Física Moderna. Universidad de Cantabria*  
Santander, 13-17 de Octubre de 1991.  
Invitado por el Departamento de Física. Profesor A. Mañanes. I
7. *Departamento d'Estructura i Constituents de la Materia. Universitat de Barcelona*  
Barcelona, 6-8 de Febrero de 1992. Profesor M. Barranco I
8. *Departamento de Física Moderna. Universidad de Granada*  
Granada, 16-18 de Marzo de 1992.  
Invitado por el Departamento de Física. Profesores J. Sánchez Dehesa y C. Recio. I
9. *Department of Physics. University of California at Berkeley*  
University of California at Berkeley (UCB), California, USA. Octubre 1992-Septiembre 1994. Profesor Marvin L. Cohen. Beca Postdoctoral Fulbright/MEC. P
10. *Department of Chemistry and Biochemistry*  
University of California at Los Angeles (UCLA), California, USA. 29-31 Enero 1993.  
Invitado por el Department of Chemistry and Biochemistry. Profesor M.A. El Sayed I
11. *Department of Chemistry*  
Duke University, Durham, North Carolina, USA. 8-15 Mayo 1993  
Invitado por el Department of Chemistry. Profesor Weitao Yang. I
12. *Department of Physics*  
Tulane University, New Orleans, Louisiana, USA. 28 Julio - 1 Agosto 1993  
Invitado por el Department of Physics y ayuda del "CIES". Profesor John Perdew. I
13. *Department of Physics. University of California at Berkeley*  
University of California at Berkeley (UCB), California, USA. Octubre 1994 - Diciembre 1994.  
Profesor Marvin L. Cohen. National Science Foundation Fellow. P
14. *Department of Physics. University of California at Berkeley*  
University of California at Berkeley (UCB), California, USA. 15-26 Marzo 1995. Invitado por los Profesores Marvin L. Cohen y Steven G. Louie. I
15. *Institut Romand de Reserche Numérique en Physique des Matériaux (IRRMA)*  
Lausanne, Suiza. 16-23 Abril-1995. Invitado por el Profesor Roberto Car. I
16. *Department of Physics. University of California at Berkeley*  
University of California at Berkeley (UCB), California, USA. Junio-Julio 1995. Invitado por los Profesores Marvin L. Cohen y Steven G. Louie, y Beca de Movilidad del Personal Investigador de la Universidad de Valladolid. I
17. *Institut Romand de Reserche Numérique en Physique des Matériaux (IRRMA)*  
Lausanne, Suiza. Septiembre-1995. Invitado por el Profesor Roberto Car. I
18. *Departamento de Física, Universidad de Coimbra*  
Coimbra, Portugal. 22-24 Noviembre 1995. Invitado por el Profesor C. Fiolhais I
19. *Department of Physics. University of California at Berkeley*  
University of California at Berkeley (UCB), California, USA. June 1996.  
Invitado por el Profesor Steven G. Louie. I
20. *Laboratoire des Solides Irradiés, Ecole Polytechnique*  
Palaiseau, Paris. Francia. 27-30 Diciembre 1996.  
Invitado por la Profesora Lucia Reining. I
21. *Department of Physics. University of York. U.K.*  
York, 23 al 27 del Julio, 20 al 26 de Septiembre 1997, Marzo 1998.  
Acciones Integradas entre España y el Reino Unido, Profesor Rex W. Godby. O



22. *Groupe de Dynamique des Phases Condenses*  
 Université de Montpellier II, Montpellier, Francia. 4-8 Febrero 1998.  
 Invitado por el Profesor Patrick Bernier y TMR-network NAMITECH. IO
23. *Departamento de Física de Materiales*  
 Universidad del País Vasco, San Sebastián. Abril-Septiembre 1998  
 Profesor Invitado Iberdrola (Grupo del Profesor Pedro M. Echenique). I
24. *Institute for Nuclear Theory, INT-98*  
 University of Washington, Seattle, Washington (USA). 3-12 Julio 1998.  
 Invitado por los Profs. G.F. Bertsch, R.S. Berry y A. Bulgac I
25. *Institute for Nuclear Theory, INT-98*  
 University of Washington, Seattle, Washington (USA). Diciembre 1999.  
 Invitado por el Prof. G.F. Bertsch I
26. *Laboratoire des Solides Irradiés, Ecole Polytechnique*  
 Palaiseau, Paris. Francia. Noviembre-2000, Febrero-2001.  
 Estancia sabática dentro del Programa Salvador de Madariaga del MEC e invitado por la Profesora Lucia Reining. IO
27. *Institut für Theoretische Physik* Freie Universität Berlin, Berlin, Germany. Noviembre 2002  
 Invitado por el Prof. E.K.U. Gross I
28. *Institut für Theoretische Physik and Fritz-Haber-Institut der Max-Planck-Gesellschaft* Freie Universität Berlin, Berlin, Germany. Junio-2005-Marzo 2006  
 Invitado por los Profs. E.K.U. Gross and M. Scheffler I
29. *Dipartimento di Fisica*  
 Università di Roma 'Tor Vergata', April 2007  
 Invitado por el Prof. R. Del Sole I
30. *nanoNMR group, LCVN, UMR5587 CNRS UM2*  
 Universidad de Montpellier 2, Francia, June-July (2007) I
31. *Departamento de Física, Universidad de Coimbra*  
 Coimbra, Portugal. Abril 2008. Invitado por el Profesor F. Noguiera I
32. *Institut für Theoretische Physik* Freie Universität Berlin, Berlin, Germany. Julio/Agosto 2008  
 Invitado por Prof. E.K.U. Gross I
33. *Fritz-Haber-Institut der Max-Planck-Gesellschaft* Berlin, Germany. June-Agosto 2009  
 Invitado por el Prof. M. Scheffler y Prof. E.K.U. Gross I
34. *UC Santa Barbara, Kavli Institute for Theoretical Physics*  
 KITP Program: Excitations in Condensed Matter: From Basic Concepts to Real Materials (October 5 - December 18, 2009) Coordinators: Claudia Ambrosch-Draxl, Kieron Burke, Roberto Car, Matthias Scheffler  
 Santa Barbara, USA Oct-Nov 2009. I
35. *Fritz-Haber-Institut der Max-Planck-Gesellschaft* Berlin, Germany. June-August 2010, 2011, 2012, 2013  
 Invitado por el Prof. M. Scheffler I
36. *Department of Physics. University of California at Berkeley*  
 University of California at Berkeley (UCB), California, USA. August-September 2013.  
 Invitado por el Profesor Steven G. Louie. I

## XIV. DOCENCIA

## A. Cursos de Licenciatura

- Curso 88-89 - *Física Cuántica (3º Físicas)*  
Facultad de Ciencias. Universidad de Valladolid.
- Curso 89-90 - *Métodos Matemáticos de la Física II (3º Físicas)*  
Facultad de Ciencias. Universidad de Valladolid.
- Cursos 89-91 - *Ampliación de Mecánica Cuántica (5º Físicas)*  
Facultad de Ciencias. Universidad de Valladolid.
- Curso 91-92 - *Física Atómica, Molecular y Nuclear (5º Físicas)*  
Facultad de Ciencias. Universidad de Valladolid.
- Spring 1993 - *Introduction to Statistical and Thermal Physics.*  
Physics 112, Section 2. Department of Physics  
En substitución del Professor Marvin L. Cohen  
University of California at Berkeley. California. USA.
- Cursos 94-98 - *Física Atómica, Molecular y Nuclear (5º Físicas)*  
Facultad de Ciencias. Universidad de Valladolid.
- Cursos 95-98 - *Laboratorios Física Atómica y Nuclear (5º Físicas)*  
Facultad de Ciencias. Universidad de Valladolid.
- Cursos 99-01 - *Mecánica Cuántica (4º Químicas)*  
*Técnicas Experimentales en Física Cuántica (3º Físicas)*  
Facultad de Ciencias. Universidad de Valladolid.

## B. Cursos de Doctorado, Master y Escuelas de Postgrado

- Professor at the 3rd PIER Graduate Week, which will take place from 10-13 October 2016 in the Center for Free-Electron Laser Science on Bahrenfeld campus, Hamburg. Course on: Many-Body Correlations in Molecules and the Solid State
- Professor at the DPG Graduate Kollegue "Research TRaining Group on Quantum Mechanical Materials Modelling", (<http://www.rtg-qm3.de>) (2016-2019)
- Professor at the International Max Planck Research School for Ultrafast Imaging and Structural Dynamics (IMPRS-UFAST) ([http://www.imprs-ufast.de/index\\_eng.html](http://www.imprs-ufast.de/index_eng.html)) (dec-2014-to date)  
Focus Course: Time-dependent density-functional theory (TDDFT) and Many-Body Techniques (MBT) (July 2016).
- Profesor del programa de Doctorado con mención de calidad del MEC: "PHYSICS OF NANOSTRUCTURES AND ADVANCED MATERIALS (Master in Nanoscience)" (2007-hasta la fecha) (MEE2007-0052; MEE2011-0591)  
Asignaturas del Master impartidas:  
Excited-state properties of low-dimensional systems  
Low dimensional systems and nanostructures  
Nanostructural properties
- Coordinator of the Interuniversity Agreement (ERASMUS) program between the Università degli studi de Catania and the Universidad del País Vasco (2011-)
- Profesor "Leibniz graduate school DinL: Dynamics in new Light" (1/6/2011-30/05/2014)
- Profesor externo en el master inter-universitario en Nanociencia y Nanotecnología Molecular, coordinado por el Prof. Eugenio Coronado, Universidad de Valencia. (2007-)  
Topic: "Single-Molecule Electronics"
- "Conceptos Básicos en Física de Materiales I: Fundamentos"  
y "Conceptos Básicos en Física de Materiales II: Aplicaciones"  
Programa de Doctorado en Ciencia y Tecnología de Materiales, UPV/EHU (2002-2008)

- Curso sobre "Métodos *ab-initio* en Materia Condensada"  
Departamento de Física Fundamental. Facultad de Física. Universidad de la Laguna, Tenerife. (9-12 Junio 1997) (Curso Invitado)
- Curso sobre "Time-Dependent Density-Functional-Theory and its Applications"  
Departamento de Física de Materiales, Universidad del País Vasco, San Sebastián. (30-Junio al 4-Julio 1997) (Curso Invitado)
- Spring College on "Electronic Structure Approaches to the Physics of Materials". International Centre for Theoretical Physics (ICTP), Trieste, Italia (15 May - 9 June 2000) (Curso Invitado).
- "III Taller de Física Computacional: Aplicaciones de los Métodos Ab-Initio en Materia Condensada". Merida, Venezuela (10 al 14 de Julio del 2000) (Curso Invitado)
- "Nuevas estructuras moleculares, los nanotubos: estructuras, propiedades y aplicaciones en nanotecnología"  
VI Escuela Nacional de Materiales Moleculares, Cartagena, Murcia (21-29 Junio 2003) (Curso Invitado)
- Spring College on "Science at the Nanoscale"  
International Centre for Theoretical Physics (ICTP), Trieste, Italia (24-31 May 2004) (Curso Invitado).
- School on "Time-Dependent Density-Functional Theory and the Dynamics of Complex Systems"  
St. John's College, Santa Fe, New Mexico (USA) (5-10 June 2004) (Curso Invitado)
- School on "Time-Dependent Density-Functional Theory: Prospects and Applications",  
Benasque Center for Science, Benasque, Huesca (Spain) August 29-September 11, (2004) (Curso invitado on Applications of TDDFT)
- School on "Ab-initio methods in materials science", National Cheng Kung University, Taiwan (August 2006) (curso invitado)
- Second School on "Time-Dependent Density-Functional Theory: Prospects and Applications",  
Benasque Center for Science, Benasque, Huesca (Spain) August 27-September 11, (2006) (Cursos invitado)
- "Introduction to Molecular Electronics" IX Escuela Nacional de Materiales Moleculares, Peñíscola, (17-20 Febrero 2008) (Curso Invitado)
- EPIOPTICS School "Internatioanl School on Solid State Physics" "The optical properties of porphyrins, the light emitting proteins",  
Erice, Sicily 20-27 June 2008 (Cursos invitado)
- Third School on "Time-Dependent Density-Functional Theory: Prospects and Applications",  
Benasque Center for Science, Benasque, Huesca (Spain) August 31-September 14, (2008) (Cursos invitado)
- Hands-on tutorial on ab initio molecular simulations: Toward a First-Principles Understanding of Materials Properties and Functions  
Harnack-House, Berlin, Germany June 22 - July 1, 2009 (Curso Invitado: Response functions in low dimensional systems: from optics to transport)
- (group meeting) "Time Dependent Density Functional Theory for molecular simulation: theory and algorithms", 19-31 July 2009, Mathematics Department Fu-Berlin (Curso invitado sobre "algorithms for time propagation of TDKS equations and exchange-correlation kernels from many body theory")
- CECAM & Psi-K Summer School on Simulation Approaches to Problems in Molecular and Cellular Biology  
Organisers Paolo Carloni, Ursula Rothlisberger, Michele Parrinello  
Palacio Miramar, San Sebastián, 31-August; 5-September (2009) (Curso Invitado: "First principles description of the optical properties of biochromophores" and CHAIRPERSON)
- "XI Escuela Nacional de Materiales Moleculares", 14-19 Febrero 2010. Peñafiel. Valladolid (Curso Invitado: Respuesta electrónica de sistemas moleculares: espectroscopía y transporte en nano-estructuras y biomoléculas)

### C. Tesis de Master y Tesinas de Licenciatura dirigidas

- *Construction of a Kohn-Sham Iteration Scheme in Time-Dependent Lattice Density-Functional Theory*  
Benedikt-Sebastian Mehmel, Directors: Markus Penz and Angel Rubio, Master University of Hamburg (29th May 2019)
- *Laser Control of Topological Polaritons*  
Damian Hoffmann, Directors: Michael Sentef and Angel Rubio, Master University of Hamburg (27th November 2018)
- *Implementation of an efficient structural minimizer in Octopus: The FIRE algorithm*  
Alejandro Varas, Director: Angel Rubio, Master in nanoscience, University of the Basque Country (25 Sep 2013)
- *Non-relativistic three-body systems and finite mass effects*  
René Jestädt, Directors: H. Appel and A. Rubio, Freie Universität Berlin, Germany 7 Nov 2012
- *Study of the Electronic Structure of hexagonal Boron Nitride on metals substrates*  
Paul Giraud, Director: Angel Rubio Co-director: Elena Cannuccia Université des Sciences et Technologies Lille 1, France 17 Sep 2012
- 1. *Modeling the thermoelectric properties of hybrid graphene-boron-nitride nanoribbons: a nonequilibrium Green's function approach*  
Kaike Yang, Director: Roberto D'Agosta and Angel Rubio Master in nanoscience, University of the Basque Country (13 Jun 2012)
- 2. *Non-adiabatic effects in one-dimensional one and two electron systems: the cases of the dihydrogen cation and the dihydrogen molecules*  
Alison Crawford Uranga, Director: Dr. L. Stella, Prof. Stefan Kurth, Prof. Angel Rubio, Master in nanoscience, University of the Basque Country (14 Sep 2011)
- 3. *Linear response functions of solids within time-dependent density functional theory(TDDFT)*  
Navid Abedi Khaleidi, Director: Angel Rubio, Master in nanoscience, University of the Basque Country (14 Sep 2011)
- 4. *Optical properties of pentacene and picene*  
Jeiran Jokar , Director: Prof. Angel Rubio, Dr. Matteo Gatti , Dr. Pierluigi Cudazzo, Master in nanoscience, University of the Basque Country (14 Sep 2011)
- 5. *Modeling Molecular Electronics: Applications to Chemical Sensors*  
Iker Larraza Arocena, Director: Dr. Duncan Mowbray and Prof. Angel Rubio, Master in nanoscience, University of the Basque Country (14 Sep 2011)
- 6. *Analysis of performance and scaling of the octopus code*  
Joseba Alberdi Rodriguez, Directors: Javier Muguerza y Angel Rubio, Master in Advanced Computer Systems, University of the Basque Country (September 2010)
- 7. *Ab initio Study of the Optical Activity in Chiral Systems*  
Leonardo Andrés Espinosa Leal, Director: Angel Rubio, Master in Nanosciences, University of the Basque Country (September 2009)
- 8. *Modified Ehrenfest formalism: A new approach for large scale ab-initio molecular dynamics*  
Xavier Andrade, Tesis Suficiencia Investigadora (Noviembre 2008)
- 9. *Quantum optimal control of high-harmonic generation from molecular systems*  
Ali Akbari, Director: Angel Rubio, Nanoscience Master Thesis (Julio 2008)
- 10. *Estudio de las propiedades ópticas de sistemas biológicos mediante la teoría del funcional de la densidad dependiente del tiempo*  
Daniele Varsano, Tesina (Septiembre 2003)
- 11. *Implementación de la Teoría del Funcional Dependiente del Tiempo: Aplicación a Pequeños Agregados*  
Alberto Castro Barrigón, (Diciembre 1999) Calificación : Matrícula de Honor.  
Codirigida con el Prof. Julio A. Alonso

12. *Estudio Estructural y Dinámico de Defectos Puntuales en Si, C y SiC*  
Teodosio del Caño González (Noviembre 1999) Calificación : Matrícula de Honor.  
Codirigida con el Dr. Eduardo Hernández.
13. *Estudio Ab-initio de las Transiciones de Fase en GaN y AlN*  
Jorge Serrano Gutiérrez (Noviembre 1998) Calificación : Matrícula de Honor.  
Codirigida con el Dr. Eduardo Hernández.
14. *Estudio Teórico de la Sección Eficaz de Fotoabsorción en Agregados Bimetálicos Puros y con Impurezas*  
M<sup>a</sup>. Begoña Torres Cabrera (Julio 1993) Calificación : Sobresaliente con Honor.  
Codirigida con el Prof. Luis Carlos Balbás Ruesgas.

#### D. Tesis Doctorales dirigidas

1. *Many Electrons and the Photon Field*  
Florian Konrad Friedrich Buchholz (24rd November 2020)  
Technische Universität Hamburg, Directors: Dr. Michael Ruggenthaler and Prof. Dr. Angel Rubio  
Magna Cum Laude.
2. *An efficient ab-initio non-equilibrium Green's function approach to carriers dynamics in many-body interacting systems*  
Fabio Covito (23rd July 2020)  
Universität Hamburg, Directors: Prof. Dr. Daniela Pfannkuche and Prof. Dr. Angel Rubio  
Magna Cum Laude.
3. *Mixed Quantum-Classical Dynamics in Cavity Quantum Electrodynamics*  
Norah Hoffmann (2nd June 2020)  
Universität Hamburg, Directors: Prof. Dr. Angel Rubio and Prof. Dr. Neepa Maitra  
Magna Cum Laude.
4. *On the interface of quantum electrodynamics and electronic structure theory: Cavity QED*  
Christian Schaefer (13th May 2020)  
Universität Hamburg, Directors: Prof. Dr. Angel Rubio and Dr. Michael Ruggenthaler  
Magna Cum Laude.
5. *Novel Approaches in Quantum Chemistry: Self-Consistent Density-Functional Embedding and Polaritonic Coupled-Cluster Theory*  
Uliana Mordovina (22nd April 2020)  
Universität Hamburg, Directors: Prof. Dr. Daniela Pfannkuche and Prof. Dr. Angel Rubio  
Magna Cum Laude.
6. *Numerical simulations for the nonequilibrium control of quantum materials*  
Gabriel Topp (22nd April 2020)  
Universität Hamburg, Directors: Dr. Michael Sentef and Prof. Dr. Angel Rubio  
Magna Cum Laude.
7. *Fully coupled Maxwell Kohn Sham systems: electromagnetic field propagation in Schrödinger-like form and ab-initio self-consistent light-matter interactions*  
René Jestaädt (10th April 2019)  
Technische Universität Hamburg, Directors: Prof. Dr. Andreas Knorr and Prof. Dr. Angel Rubio  
  
Magna Cum Laude.
8. *Density Matrix Embedding Theory Foundations, Applications and Connection to Functional Theories*  
Teresa Reinhard (26th March 2019)  
Universität Hamburg, Directors: Prof. Dr. Daniela Pfannkuche and Prof. Dr. Angel Rubio  
  
Magna Cum Laude.

9. *Quantum Electrodynamical Time-Dependent Density Functional Theory*  
Camilla Pellegrini (21st September 2017) Director: Prof. Dr. Angel Rubio and Prof. Ilya Tokatly  
Sobresaliente Cum Laude.
10. *Modeling linear and non-linear light-matter interactions: From classical to atomistic nanoplasmonics*  
Alejandro J. Varas Barbosa (4rd September 2017) Director: Prof. Dr. Angel Rubio and Prof. Pablo García González  
Sobresaliente Cum Laude.
11. *Exact Maps in Density-Functional Theory*  
Tanja Dimitrov (9th February 2017) Technische Universität Hamburg, Directors: Prof. Dr. Andreas Knorr and Prof. Dr. Angel Rubio  
  
Magna Cum Laude.
12. *Modelling of Polymer–Carbon Nanotube Heterojunctions for Photovoltaic Applications*  
Livia Noemi Glanzmann, (31st January 2017) International PhD Thesis Directed by Duncan Mowbray and Ángel Rubio  
Sobresaliente Cum Laude
13. *Theoretical study on the photoswitching mechanism of negative reversibly photoswitchable uorescent proteins*  
Bruno Torcal Embeita (25th October 2016)  
PhD Thesis Directed by Marius Wanko and Ángel Rubio  
Sobresaliente Cum Laude
14. *Modeling and Analysis of Thermoelectric Energy Conversion Efficiency in Nanostructures*  
Kaike Yang (22nd June 2016)  
International PhD Thesis Directed by Roberto D’Agosta and Ángel Rubio  
Sobresaliente Cum Laude
15. *Modelling Thermo-Electric Transport and Excited States in Low Dimensional Systems*  
Robert Biele(17nd June 2016)  
International PhD Thesis Directed by Roberrrto D’Agosta and Ángel Rubio  
Sobresaliente Cum Laude
16. *Exact Nonadiabatic Many-Body Dynamics: Electron-Phonon Coupling in Photoelectron Spectroscopy and Light-Matter Interactions in Quantum Electrodynamical Density-Functional Theory*, Johannes Flick, (30th May 2016)  
Humboldt-Universität zu Berlin, PhD Thesis Directed by Ángel Rubio, Heiko Appel and M. Scheffler  
Magna Cum Laude
17. *Analysis and Control of Transient Spectra Using Time-Dependent Density Functional Theory*  
Jessica Walkenhorst (29th January 2016)  
International PhD Thesis Directed by Alberto Castro and Ángel Rubio  
Sobresaliente Cum Laude
18. *Density-potential mapping in the standard and quantum electrodynamical time-dependent density functional theory*  
Mehdi Farzanehpour (30th October 2015)  
International PhD Thesis Directed by Ilya Tokatly and Ángel Rubio  
Sobresaliente Cum Laude
19. *Spectroscopic analysis of atoms and molecules*  
Alison Crawford Uranga (11th September 2015)  
International PhD Thesis Directed by Ángel Rubio and Stefan Kurth  
Sobresaliente Cum Laude
20. *Optimisation of the first principle code octopus for massive parallel architectures:application to light harvesting complexes*  
Joseba Alberdi-Rodriguez (4rd June 2015)  
International PhD Thesis Directed by Ángel Rubio and Javier Muguerza  
Sobresaliente Cum Laude

21. *Theoretical Description of the Optical Properties of Nanostructures Within Time Dependent Density Functional Theory*, Leonardo Andrés Espinosa Leal, (22nd October 2013)  
European PhD Thesis Directed by Ángel Rubio and Daniele Varsano  
Apto Cum Laude
22. *Self-consistent GW approach for the unified description of ground and excited states of finite systems*  
Doktor der Naturwissenschaften (Dr.rer.nat). Fachbereich Physik, Freie Universität Berlin, Fabio Caruso, (21st October 2013), Director M. Scheffler, Co-director: . Rubio  
Summa cum Laude
23. *Density-Functional Theory for f-Electron Systems: The  $\alpha - \gamma$  Phase Transition in Cerium*  
Doktor der Naturwissenschaften (Dr.rer.nat). Fachbereich Physik, Freie Universität Berlin, Marco Casadei, (21st October 2013), Director M. Scheffler, Co-director: . Rubio  
Magna cum Laude
24. *Static and time-dependent density functionals for non-linear processes*, Johanna I. Fuks, (18th June 2013),  
European PhD Thesis Directed by Ángel Rubio  
Apto Cum Laude
25. *Development and applications of time-dependent density matrix functional theory*, Ali Akbari, (27th September 2012), European PhD Thesis Directed by Ángel Rubio  
Apto Cum Laude
26. *Improving simulation of biological molecules: refining mathematical, physical and computational tools*, Pablo García Risueño, 15th December 2011, European PhD Thesis Directed by José Luis Alonso, Pablo Echenique and Ángel Rubio  
Sobresaliente Cum Laude
27. *Linear and non-linear response phenomena of molecular systems within time-dependent density functional theory*. Xavier Andrade, 8th October 2010. European PhD Thesis directed by Angel Rubio and Silvana Botti  
Sobresaliente Cum Laude y Premio extraordinario de Doctorado 2010/2011
28. *Relativistic effects in the optical response of low-dimensional structures: new developments and applications within a time-dependent density functional theory framework*. Micael Oliveira, 29-Enero-2009. Tesis cotutelada con el Profesor Fernando Nogueira (U. Coimbra)  
Sobresaliente Cum Laude
29. *First principles description of response functions in low dimensional systems* . Daniele Varsano. 13-Julio-2006.  
Sobresaliente Cum Laude y Premio extraordinario de Doctorado 2006/2007
30. *Synthèse de nanotubes de nitrure de bore: études de la structure et des propriétés (vibrationnelles et électroniques)*  
Raul Arenal de la Concha. (empezada en el 2001; cotutelada con Annick Loiseau del LEM Unité Mixte ONERA-CNRS, Paris, Francia). Cum Laude (4-Febrero-2005)
31. *Una metodología de primeros principios, basada en la teoría del funcional de la densidad dependiente del tiempo, para el cálculo de la respuesta electromagnética de nanoestructuras*. Alberto Castro Barrigón. Apto Cum Laude (13-Julio-2004)
32. *Efectos de la temperatura y la masa isotópica en las propiedades de los semiconductores: influencia en el comportamiento de los fonones y los estados electrónicos*. Jorge Serrano Gutiérrez (se leyó en Stuttgart Junio 2003)
33. *Resonancia Magnética Nuclear en Nanotubos de Carbono* Sylvain Latil. (Septiembre 2001) (codirigida con el Dr. Patrick Bernier de la Universidad de Montpellier)

**E. Supervisión de Becarios Postdoctorales y Sabáticos**

1. Dr. Zahra Nourbaksh, Postdoctoral Researcher SOLSTICE (DFG) (July-2019-)
2. Dr. Dominik Sidler, Postdoctoral Researcher RouTE (QuanTER-EC) (June-2019-)
3. Dr. Jin Zhang, Postdoctoral Researcher MPSD (July-2017-)
4. Dr. Emil Vinas Boström, Postdoctoral Researcher MPSD (May-2019-)
5. Dr. Dongbin Shin, Korean postdoctoral fellow (Sept. 2019-); Postdoctoral Researcher MPSD (March-2019-August 2019)
6. Dr. Franco Bonafe, Postdoctoral Researcher MPSD (Feb-2019-)
7. Dr. Martin Lüders, Technician MPSD (2019-)
8. Dr. Shunsuke Sato, AvH Postdoctoral Researcher MPSD (April-2016-May-2019) and hosting in Hamburg his Tenure Track Assistant Professor position at Tsukuba University in Japan (May-2019-)
9. Dr. Oleg Kristanvoski, Postdoctoral Researcher MPSD (Feb 2019- Dec 2019)
10. Dr. Julian Gebhardt, Guest DFG Postdoc MPSD (2018-Mayo 2019)
11. Dr. Peizhe Tang, MPSD Postdoc ((Nov-2017- May-2018) and Marie Curie Actions- Individual Fellowships (IF) (May-2018-2020)
12. Dr. Derrien Thibault, Postdoc MPSD (March 2018-2019)
13. Dr. Joaquim Sornet Somoza, Beatriu de Pinós fellowship, Montpellier-Donostia (December 2012-2014); Juna de la Cierva (Oct. 2015-2018), Marie Curie Actions- Individual Fellowships (IF) (Oct-2018-)
14. Dr. Markus Penz, Schrödinger Fellow Austrian Science Foundation (October-2017-)
15. Dr. Wenjuan Yang, Postdoctoral Researcher MPSD (October-2017-September 2019)
16. Dr. José J. Baldovi, Marie Curie Intra European Fellowship (IEF) (Oct-2017-Srp. 2019); Postdoctoral Researcher UPV/EHU- ERC (Jan-September 2017)
17. Dr. Guillermo Albareda, Marie Curie Intra European Fellowship (IEF) (Oct-2017-2019)
18. Dr. Enrico Ronca, Postdoctoral Researcher MPSD (September-2017-)
19. Dr. Simone Latini, Postdoctoral Researcher MPSD (March-2017-)
20. Dr. Micael Oliveira, Technician MPSD (2016-)
21. Dr. Nikko Säkkinen, Postdoctoral Researcher MPSD (March-September 2017)
22. Dr. Florian Eich, Marie Curie Intra European Fellowship (IEF) (Oct-2016-Dec.2019); Postdoctoral fellow MPSD (Oct-2015-Sept-2016)
23. Dr. Cesar A. Rodriguez-Rosario, Marie Curie Intra European Fellowship (IEF) (April-2016-MArch 2018)
24. Dr. Aaron T. Kelly, Postdoctoral Researcher MPSD (March-2016-June-2017)
25. Dr. Juan Borje, Marie Curie Intra European Fellowship (IEF) (May-2016-); Postdoctoral Fellow (March-2015-April-2016)
26. Dr. Ali Abedi, Marie Curie Intra European Fellowship (IEF) (May-2016-); Postdoctoral Fellow (Jan-2015-April-2016)
27. Dr. Elham Khosravi, Marie Curie Intra European Fellowship (IEF) (May-2016-); Postdoctoral Fellow (Jan-2015-April-2016)
28. Dr. Andrea Droghetti, Contrato Juan de la Cierva (octubre 2014-2015); Marie Curie Intra European Fellowship (IEF) (2016-2019)



29. Dr. Nicolas Tancogne-Dejean, Contrato postdoctoral MPSD (Jan-2016-)
30. Dr. Henning Glawe, Contrato postdoctoral-NOMAD MPSD (Nov-2015-)
31. Dr. Soren Nielsen, Contrato postdoctoral MPSD (Nov-2015-2018)
32. Dr. Iris Theophilou, Contrato postdoctoral MPSD (Oct-2015-)
33. Dr. Arun Debnath, Contrato postdoctoral MPSD (Sep-2015-May 2019)
34. Dr. Thomas Brumme, Contrato postdoctoral MPSD (Sep-2015-2017)
35. Dr. Michael Ruggenthaler, Contrato postdoctora Senior MPSD (Sep-2015-)
36. Dr. Adriel Dominguez, Contrato postdoctoral MPSD (Jun-2015-2019)
37. Dr. Michael Sentef, Contrato postdoctoral MPSD (Apr-2015-2016)
38. Dr. Lede Xian, Contrato Postdoctoral (Jan-2014-March 2017); Marie Curie International Fellowships (H2020- MSCA-IF-2016) (2017-2019)
39. Dr. Umberto de Giovannini, Contrato postdoctoral MPSD (Jan-2017-); Contratado Postdoctoral UPV/EHU (2010-2016)
40. Dr. Heiko Appel, Contrato postdoctoral MPSD (March-2015-); FHI-postdoc (2010-2015)
41. Dr. Hannes Huebner, Contrato postdoctoral MPSD (Oct-2016-); Marie Curie Intra European Fellowship (IEF) (Oct-2014-2016)
42. Dr. Ask Hjorth Larsen, Contrato Postdoctoral (March-2012-2019)
43. Dr. Philipp Wopperer, Contrato Postdoctoal (Junio-2014-2017)
44. Dr. Stefan Kurth, Profesor Ikerbasque, (Octubre 2008 -)
45. Dr. Ilya Tokatly, Profesor Ikerbasque, (Diciembre 2007-)
46. Dr. Roberto D'Agosta, Contratado Postdoctoral del Proyecto FANCYNANO (19-Noviembre-2008;31-Marzo-2009); Profesor Ikerbasque (Abril 2009-)
47. Dr. Ravindra Laxman Shinde, Contrato Postdoctoral (Setp-2014-Oct-2015)
48. Dr. Sener Sen, Contrato Postdoctoral (5-May-2014-June 2017)
49. Dr. Seymour Cahangirov, JAE-doc CSIC (Sep-2012-March 2013); Marie Curie (April 2014-Aug-2015)
50. Dr. Alejandro Pérez Paz, Contratado Postdoctoral (Oct-2010-Abril 2017)
51. Dr. Irina V. Lebedeba, Contratado Postdoctoral DYNAPLEX (Oct-2012-June-2013); Marie Curie Actions-International Incoming Fellowships (IIF) (FP7-PEOPLE-2012-IIF, Project: 326435) (June-2013-May-2015)
52. Dr. Guillermo Albareda, Beatriu de Pinos fellowship FHI-Berlin (April 2012-2014)
53. Dr. Victor Morón Tejero, Contratado Postdoctoral UPV/EHU (Oct-2012-2014)
54. Dr. David Cardamone, Contrato Postdoctoral (Oct-2011-Dec-2014)
55. Dr. Duncan Mowbray, DIPC Postdoc (15-Noviembre-2009-April-2011); Juan de la Cierva (April-2011-March 2014); GV Postdoc (April-Dec 2014)
56. Dr. Marius Wanko, Consolider postoc (2009-2010); Juan de la Cierva (January-2011-Dec.-2013); GV Postdoc (Jan-2014-2015)
57. Dr. Yann Pouillon, Becario Postdoctoral del Programa Europeo IST, SANES (Sep.-2006, Dic.2008), Técnico doctor (2009-2016)
58. Dr. Amilcare Iacomino, JAE-doc CSIC (May 2010,-Nov. 2013)

59. Dr. Daniel Rohr Marie Curie Actions-Intra-European Fellowships (IEF) ( FP7-PEOPLE-2011-IEF, Project: 302603) (April-2013-March-2015)
60. Dr. Ermin Malic Fritz-Haber-Institut Max-Planck-Gesellschaft, Berlin (Germany) (Jan-2013-Apr-2013)
61. Dr. Elena Cannuccia, Contratado Postdoctoral (June-2011-January 2013)
62. Dr. Annapaola Migani. JAE-doc CSIC (Sep-2010-Dic.-2012)
63. Dr. Lorenzo Stella, Contratado Postdoctoral UPV/EHU (Sep-2010-Jan.2013)
64. Dr. Matteo Gatti, Contratado Juan de la Cierva, Enero 2009-2011, Postdoc Grupos Consolidados (2012).
65. Dr. Federico Iori, Contratado Postdoctoral (Sep-2010-Apr-2011); Postdoc UPV/EHU (May 2011- Nov. 2011)
66. Dr. Jose Luis Cabellos Quiroz, Postdoc del Gobierno Mexicano (Dec-2010-Dec-2011)
67. Dr. Claudio Attacalite, Contratado Juan de la Cierva, Diciembre 2007-2010
68. Dr. Juan Maria Garcia-Lastra, Contratado Juan de la Cierva, Dic. 2006-2009; Contratado Postdoctoral del Proyecto Europeo THEMA-CNT (Dic.-2009-Dic.2010)
69. Dr. Pierluigi Cudazzo, Contratado Postdoctoral del Proyecto FANCYNANO (1-Junio-2009-August 2014) y ERA-CHEMISTRY (10-Febrero-2009;30-Mayo-2009)
70. Dr. Letizia Chiodo Contratada Postdoctoral del Proyecto Europeo NANO-ERA Chemistry(15-June;Octubre-2008) y Postdoc UPV/EHU ( 1-Noviembre-2008-31-Enero-2010)
71. Dr. Nicole Helbig, Contrato Postdoctoral asociado a NANOQUANTA/ETSF, November-2007,Diciembre 2010.
72. Dr. Matthieu Verstrete, Contratado Postdoctoral del Proyecto Europeo NANO-ERA Chemistry (May-2008; Agosto 2009)
73. Dr. Kristian Sommer Thygesen, Becario Postdoctoral del Programa Europeo IST, SANES (Sept-2005, Sept-2006)
74. Dr. Michel Bockstedte, DFG-postdoctoral fellowship (Abril-2005, Diciembre 2006)
75. Dr. Francesco Sottile, Becario Postdoctoral de la Red de Excelencia NANOQUANTA (Nov-2004, Apr-2006)
76. Dr. Mathieu Dubois, Beca Postdoctoral, (Enero-Febrero 2005)
77. Dr. Myrta Gruening: Contrato Postdoctoral del DIPC (Noviembre-2003-Diciembre 2005)
78. Dr. Ludger Wirtz: Contrato Postdoctoral del Programa Europeo RTN, COMELCAN (Febrero-2002,Diciembre-2004)
79. Dr. Andrea Marini: Contrato Postdoctoral del Programa Europeo RTN, NANOPHASE (Junio-2002,Junio-2004)
80. Dr. François Triozon: Becario Postdoctoral del Programa Europeo RTN, COMELCAN (Septiembre-2002,Febrero-2003)
81. Dr. Miguel Marques: Contrato Postdoctoral del Programa Europeo RTN, NANOPHASE (Junio-2000,Diciembre-2002)
82. Dr. Franck Rabilloud: Contrato Postdoctoral del Programa Europeo RTN, COMELCAN (Enero-2001,Octubre-2001)
83. Dr. Stephan Roche: Contrato Postdoctoral del Programa Europeo TMR, NAMITECH (Agosto-1999,Septiembre-2000)
84. Dr. Juan Arellano, Universidad de Valladolid (1999-2000)
85. Dr. Eduardo Hernández: Contrato Postdoctoral del Programa Europeo TMR, NAMITECH (Febrero-1997,Enero-1999).

86. Dr. Christophe Goze. Estancia de Doctores Comunitarios en España dentro del Programa Europeo TMR, NAMITECH (Julio-Agosto 1997)
87. Dr. Ihsam Boustani: Estancias de Investigadores Extranjeros en Régimen de año sabático. Programa Sectorial de Promoción del Conocimiento, Ministerio de Educación y Ciencia. Ref. SAB95-0670 (Enero-Junio 1998; Febrero-Julio 1999).
88. Oleg Gritsenko, Cátedra BBVA (1998)
89. José M. Cabrera Trujillo, Universidad de Valladolid (1994-1995).

#### **F. Supervisión de Becarios Predoctorales**

1. Matteo Vandelli, PhD Student (AIM Cluster, MPSD-Hamburg, IMPRS) (15-1-2019;-)
2. Lukas Windgätter, PhD Student (SFB925, MPSD-Hamburg, IMPRS) (1-6-2018; )
3. Damian Hofmann, PhD Student (MPSD-Hamburg, IMPRS) (1-12-2018;-)
4. Kevin Lively, PhD Student (MPSD-Hamburg, IMPRS) (1-10-2018;-)
5. Mona Kalthoff, PhD Student (MPSD-Hamburg, IMPRS) (1-10-2018;-)
6. Chang-Ming Wang, PhD Student (MPSD-Hamburg, IMPRS) (1-9-2017;-)
7. Mary-leena Tchenkoue, PhD Student (MPSD-Hamburg, IMPRS) (1-9-2017;-)
8. Alexandra Gobel, PhD Student (MPSD-Hamburg, IMPRS) (1-6-2017;-)
9. Vasil Rokaj, PhD Student (MPSD-Hamburg, IMPRS) (1-12-2016;-)
10. Davis Welakuh, PhD Student (MPSD-Hamburg, IMPRS) (15-9-2016;-)
11. Gabriel Topp, PhD Student (MPSD-Hamburg, IMPRS) (1-12-2015;-)
12. Fabio Covito, PhD Student (MPSD-Hamburg, IMPRS) (1-11-2015;-)
13. Christian Schaefer, PhD Student (MPSD-Hamburg, IMPRS) (1-11-2014;-)
14. Nora Hoffmann, PhD Student, (MPSD-Hamburg, IMPRS) (1-1-2015;31-12-2019)
15. Florian Buchholz, PhD Student, (MPSD-Hamburg) (4-1-2015;-)
16. Uliana Mordovina, PhD Student, (MPSD-Hamburg, IMPRS) (1-11-2014;-)
17. Teresa Reinhard, PhD Student, (MPSD-Hamburg, IMPRS) (1-12-2014;31-May-2019)
18. Tanja Dimitrov, PhD Student (FHI + MPSD ) (2011-2017)
19. René Jöstadt, Becario ERC (1-Ago-2013-May-2014); MPG-PhD (June 2014-July 2019)
20. Alejandro Varas, Becario ERC-DYNamo (15-Feb-2013-Dec-2017)
21. Camila Pellegrini, Becaria ERC-DYNamo, (26-Nov-2012-30-Sep-2017)
22. Kyung-Min Lee, PhD Student (MPSD-Hamburg, IMPRS) (27-8-2015-30-7-2017)
23. Raison Dzousa, PhD Student (MPSD-Hamburg, IMPRS) (15-9-2015;1-11-2016)
24. Livia Noemi Glanzmann, Marie Curie Fellowship (ITN-POCAONTAS) (20-May-2013Dec-2016)
25. Johannes Flick, PhD Student (FHI + MPSD ) (2011-2016)
26. Robert Biele becario Consolider NanoTherm (2011-2017)

27. Kaike Yang, becario Consolider NanoTherm (2011-2016)
28. Bruno Torcal Embeita, becario FPI (Dynaplex) (oct-2011-2016)
29. Jessica Walkenhorst, becaria UPV (2010-2016)
30. Jean-Pierre Inchaustegui, Master Student, (MPSD-Hamburg) (9-2-2015;2016)
31. Mehdi Farzanehpour, becario UPV (2011-2015)
32. Alison Crawford Uranga, becaria GV (2010-2015)
33. Joseba Alberdi, becario UPV/EHU (2010-2015)
34. Fulvio Berardi, becario CSIC (2009-2014)
35. Martin Madel, Becario ERC-DYNamo, (26-Nov-2012-5-May-2014)
36. Marco Casadei, FHI-fellow (Jan-2009-Apr. 2014)
37. Fabio Caruso, FHI-fellow (Jan-2009-Dec-2013)
38. Johanna Fuks, Becaria asociada al proyecto FANCYNANO del MEC (3-Noviembre-2008-Junio 2013)
39. Peizhe Tang, Tsinghua University, Beijing P.R.China (Oct-2012-Apr-2013)
40. Paul Giraud Universite de Lille, France (April-September 2012)
41. Leonardo Andres Espinosa Leal, Becario asociado al Proyecto Europeo NANO-ERA Chemistry; (Octubre 2007-Junio 2008); CSIC fellow (July-2008-Dec-2012)
42. Ali Akbari, Becario asociado al Proyecto Europeo DNA-NANODEVICES y NANO-ERA Chemistry; (Agosto 2006-Junio-2008); CSIC Fellow (July 2008-Dec-2012)
43. Xavier Andrade, Becario Marie Curie del Proyecto Europeo NANOQUANTA e ETSF, Tesis codirigida con S. Botti y M.A.L. Marques (Apr.2005- Dec.2010)
44. Micael Oliveira, Becario del Gobierno Portugues (2003-2008), Tesis cotutelada con el Profesor Fernando Nogueira de la Universidad de Coimbra, Portugal.
45. Sebastien Le Roy, Stage from Ecole Polytechnique, France (May-July 2006)
46. Daniele Varsano, Becario de la Comunidad Europea asociado al Proyecto COMELCAN (2001-2003), y NANOQUANTA (2004-2005)
47. Raul Arenal de la Concha, Becario de la Comunidad Europea asociado al Proyecto COMELCAN (2001-2003) Tesis cotutelada con la Profesora Annick Loiseau (ONERA- CNRS-U. Paris-Sud XI, Francia)
48. Alberto Castro, Beca de Colaboración de la Universidad de Valladolid (1999); Becario Predoctoral del Subprograma de Formación de Profesorado Universitario del MEC (2000-2004).
49. Sylvain Latil, Becario asociado al Proyecto NAMITECH, Universidad de Montpellier (1999-2001)
50. Jorge Serrano Gutiérrez, Beca de Colaboración MEC (1998); Becario Predoctoral del Subprograma de Formación de Profesorado Universitario del MEC (1999-2001).
51. Teodófilo del Caño González, Beca de Colaboración de la Universidad de Valladolid (1998); Beca de Colaboración MEC (1999).

## XV. OTROS MÉRITOS

## A. Artículos más citados (con más de 150 citas)

1. G. Onida, L. Reining y A. Rubio  
*Electronic excitations: density-functional versus many-body Green's-function approaches*  
Reviews of Modern Physics **74** 601-659 (2002) 1050 cites
2. A. Rubio J.L. Corkill y M.L. Cohen,  
*Theory fo graphitic BN annotubes*  
Physical Review (Rap. Comm.) B **49**, 5081-5084 (1994) 871 cites
3. P.M. Ajayan, L.S. Schadler, C. Giannaris y A. Rubio  
*Single-walled carbon nanotube-polymer composites: Strength and weakness*  
Advanced Materials **12**, 750-753 (2000) 868 cites
4. X. Blase, A. Rubio, S. G. Louie y M. L. Cohen,  
*Stability and band-gap constancy of boron-nitride nanotubes*  
Europhysics Letters **28**, 335-340 (1994) 815 cites
5. E. Hernández, C. Goze, P. Bernier y A. Rubio,  
*Elastic properties of C and BxCyNz composite nanotubes*  
Physical Review Letters **80**, 4502 (1998) 784 cites
6. D. Sánchez-Portal, E. Artacho, J.M. Soler, A. Rubio y P. Ordejón  
*Elastic properties of C and BxCyNz composite nanotubes*  
Physical Review B **59**, 12678-12688 (1999). 565 cites
7. A. Mujica, A. Rubio, A. Muñoz y R. J. Needs,  
*High-pressure phases of group-IV, III-V, and II-VI compounds*  
Reviews of Modern Physics **75** 863-912 (2003) 376 cites
8. P.J. Britto, K.S.V. Santhanam, A. Rubio, J.A. Alonso y P.M. Ajayan  
*Improved charge transfer at carbon nanotube electrodes*  
Advanced Materials **11**, 154-157 (1999) 358 cites
9. Z. Weng-Sieh, K. Cherrey, N.G. Chopra, X. Blase, Y. Miyamoto, A. Rubio, M.L. Cohen, R. Gronsky, S.G. Louie y A. Zettl,  
*Synthesis of BxCyNz nanotubes*  
Physical Review (Rap. Comm.) B **51**, 11229 (1995) 294 cites
10. A. Rubio, J.L. Corkill, M.L. Cohen, E.L. Shirley y S.G. Louie  
*Quasiparticle bandstructure of AlN and GaN*  
Physical Review B **48**, 11810-11816 (1993) 292 cites
11. J.M. Nugent, K.S.V. Santhanam, A. Rubio y P.M. Ajayan  
*Fast electron transfer kinetics on multiwalled carbon nanotube microbundle electrodes*  
Nano Letters **1**, 87-91 (2001) 290 cites
12. M.A.L. Marques, A. Castro, G.F. Bertsch and A. Rubio  
*Octopus: a first-principles tool for excited electron-ion dynamics*  
Computer Physics Communications **151/1** 60-78 (2003) 263 cites
13. Y. Miyamoto, A. Rubio, M.L. Cohen y S.G. Louie,  
*Chiral tubes of hexagona BC2N*  
Physical Review B **50**, 4976 (1994) 256 cites
14. X. Blase, A. Rubio, S. G. Louie y M. L. Cohen,  
*Quasi-particle band-structure of bulk hexagonal boron-nitride and related systems*  
Physical Review B **51**, 6868-6875 (1995) 240 cites

15. P.M. Echenique, J.M. Pitarke, E.V. Chulkov and A. Rubio  
*Theory of inelastic lifetimes of low-energy electrons in metals*  
Chemical Physics **251**, 1-35 (2000). 237 cites
16. V.H. Crespi, M.L. Cohen y A. Rubio,  
*In situ band gap engineering of carbon nanotubes*  
Physical Review Letters **79**, 2093-2096 (1997) 227 cites
17. A. Castro, M.A.L. Marques, H. Appel, M. Oliveira, C.A. Rozzi, X. Andrade, F. Lorenzen, E.K.U Gross and A. Rubio  
*octopus: a tool for the application of time-dependent density functional theory*  
Physica Status Solidi (b) **243** 2465-2488 (2006) 221 cites
18. C. Gómez-Navarro, P.J. de Pablo, J.Gómez-Herrero, B.Biel, F.J. Garcia-Vidal, A. Rubio, and F. Flores,  
*Tuning the conductance of single-walled carbon nanotubes by ion irradiation in the Anderson localization regime*  
Nature Materials **4** 534-539 (2005) 219 cites
19. J. Serrano, A.H. Romero, F.J. Manjón, R. Lauck, M. Cardona and A. Rubio  
*Pressure dependence of the lattice dynamics of ZnO: An ab initio approach*  
Physical Review B **69** 094306-1,14 (2004) 194 cites
20. O. Zakharov, A. Rubio, X. Blase, M.L. Cohen y S.G. Louie  
*Quasi-particle band structures of 6 ii-vi-compounds - ZNS, ZNSE, ZNTE, CDS, CDSE, AND CDTE*  
Physical Review B **50**, 10780 (1994) 189 cites
21. E. Hernández, C. Goze, P. Bernier y A. Rubio,  
*Elastic properties of single-wall nanotubes*  
Applied Physics A **68** 287-292 (1999) 174 cites
22. Y. Miyamoto, A. Rubio, M.L. Cohen y S.G. Louie,  
*Electronic-properties of tubule forms of hexagonal BC3*  
Physical Review B **50** 18360 (1994) 168 cites
23. J.N. Coleman, A.B. Dalton, S. Curran, A. Rubio, A.P. Davey, A. Drury, B. McCarthy, B. Lahr, P.M. Ajayan, S. Roth, R.C. Barklie and W.J. Blau,  
*Phase separation of carbon nanotubes and turbostratic graphite using a functional organic polymer*  
Advanced Materials **12**, 213-216 (2000) 162 cites
24. S. Kurth, G. Stefanucci, C.-O. Almbladh, A. Rubio and E.K.U. Gross  
*Time-dependent quantum transport: A practical scheme using density functional theory*  
Physical Review B **72** 035308-1,13 (2005) 160 cites
25. A. Rubio, D. Sánchez-Portal, E. Artacho, P. Ordejón y J.M. Soler  
*Electronic states in a finite carbon nanotube: A one-dimensional quantum box*  
Physical Review Letters **82**, 3520-3523 (1999). 150 cites
26. Y. Miyamoto, A. Rubio, X. Blase, M.L. Cohen y S.G. Louie  
*Ionic cohesion and electron doping of thin carbon tubules with alkali atoms*  
Physical Review Letters **74**, 2993-2996 (1995) 150 cites

- En total más de 28000 citas: Índice h=84.

- ISI Essential Science Indicators in Physics, Chemistry and Materials Science (<http://isiknowledge.com>).

- El trabajo "Direct Imaging of Covalent Bond Structure in Single-Molecule Chemical Reactions", Science 340, 1434 - 1437 (2013) ha sido objeto de un Perspective Chemistry Seeing the Reaction Franz J. Giessibl Science 21 June 2013: 1417-1418

Los trabajos A. Rubio *et al.* Physical Review Letters **77**, 247-250 (1996) y X. Blase *et al.* Physical Review (Rapid Communications) B **52**, 2225 (1995) han sido objeto de un "Perspectives in Science: Condensed Matter Physics", Science **273**, 751 (1996).

Los trabajos A. Rubio *et al.* Physical Review B **49**, 5081-5084 (1994); **53**, 4023-4026 (1996) han sido destacados en Science **280**, 545 (1998) (Applied Physics: "Nanowires: Small is Beautiful").

- The work G. Gao et al, Nano Letters **12**, 3518 - 3525 (2012) *Artificially stacked of two-dimensional atomic layers: towards new van der Waals solids* was *Highlighted in Nature Nanotechnology* **7**, 481 (2012) "Mix and Match"
- El trabajo C. Gómez-Navarro *et al*, ha sido destacado con un News and Views en el mismo número de Nature Materials ( Vol.4, pag. 514-515) y seleccionado por el ISI como "hot paper in materials science" (Noviembre 2006),
- The work *Ab initio electronic and optical spectra of free-base porphyrins: the role of electronic correlation* Journal of Chemical Physics **131**, 084102-1,7 (2009) has been identified on the list of our Top 20 Most Downloaded Articles in September 2009.
- Los siguientes trabajos han sido seleccionados como **portada** de sus correspondientes revistas: *Hybridized Graphene: Nanoscale patchworks* Nature Materials **9**, 379-380 (2010); *Absorption Spectra of p-Nitrophenolate Anions in Vacuo and in Solution* ChemPhysChem **10** 1207-1209 (2009) ; *Ab initio electronic and optical spectra of free-base porphyrins: the role of electronic correlation* Journal of Chemical Physics **131**, 084102-1,7 (2009); and *The challenge of predicting optical properties of biomolecules: what can we learn from time-dependent density-functional theory*. Comptes Rendus Physique **10** 469-490 (2009)
- Los siguientes trabajos han sido seleccionados como "Editor's Suggestions in Physical Review": *Quantum electrodynamical Bloch theory with homogeneous magnetic fields* Physical Review Letters (2019); *Impact of the electronic band structure in high-harmonic generation spectra of solids*, Physical Review Letters **118**, 087403 (2016); *Optimized Effective Potential for Quantum Electrodynamical Time-Dependent Density Functional Theory* Physical Review Letters **115**, 093001 (2015); *Quantum Electrodynamical Density-Functional Theory: Bridging Quantum Optics and Electronic-Structure Theory*, Physical Review A **90** 012508-1,26 (2014); *The role of non-local exchange in the electronic structure of correlated oxides*, Physical Review B **85** 115129-1,10 (2012); *Hot electron assisted femtochemistry at surfaces - a TDDFT approach* Physical Review B **79** 195405-1,10 (2009) *Electronic structure and electron-phonon coupling of doped graphene layers in KC<sub>8</sub>* Physical Review B **79** 205106-1,9 (2009) *Angle-resolved photoemission study of the graphite intercalation compound KC<sub>8</sub>: A key to graphene* Physical Review B **80**, 075431-1,5 (2009). This one was *Highlighted with a Synopsis on the Physics website: "Dirac Cone Revealed"* (<http://physics.aps.org>); *Sodium: a charge-transfer insulator at high pressures* Physical Review Letters (2010) and also *Highlighted with a Synopsis on the Physics website: "Pressure dulls shiny metals"* (<http://physics.aps.org>)
- The work *Unraveling the Intrinsic Color of Chlorophyll* published in *Angewandte Chemie* (2015) has been selected as a Hot Paper in Photosynthesis.
- Varios trabajos han sido destacados en nanotechweb.org (from the Institute of Physics Publishing that serves the global nanotechnology community) y en el "Virtual Journal of Nanoscale Science and Technology" (<http://www.vjnano.org>).
- El código OCTOPUS (<http://www.tddft.org/programms/octopus>) que se ha desarrollado en colaboración con M.A.L. Marques, A. Castro y G.F. Bertsch y que hoy en día es utilizado por más de trescientos grupos de investigación en todo el mundo debido a su eficacia.
- El trabajo *Electronic Excitations: Density-Functional versus Many-body Green's-Functions Approaches*, by G. Onida, L. Reining and A. Rubio, in *Reviews of Modern Physics* **74** 601-659 (2002); ha sido seleccionado como uno de los artículos importantes de la física en los últimos años (ver ISI Essential Science Indicators). El 9 de Septiembre del 2008 Thomson Reuters' Essential Science Indicators lo ha seleccionado como uno de los artículos más citados en física (see <http://ScienceWatch.com>).

**B. Idiomas**

(R = regular, B = bien, C = correctamente)

IDIOMA	HABLA	LEE	ESCRIBE
Inglés	C	C	C
Italiano	B	C	C
Francés	R	C	R

**C. Sociedades de Física a las que pertenece**

- Socio numerario de la *Real Sociedad Española de Física*. Madrid, 10-Enero-1992.
- Miembro de la Asociación Alexander von Humboldt, 2006-
- Miembro de la "American Association for The Advancement of Science (AAAS), Julio-1994
- Miembro de la "American Physical Society (APS)". 1-Julio-1993
- Miembro de la "American Chemical Society (ACS)". 15-May-2013
- Miembro de la "European Physical Society (EPS)". January-2016

**D. Actuación como evaluador:**

- Member of the External Scientific Advisory Board of CIQUIS ("Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares") Universidade de Santiago de Compostela (USC) (2017-)
- Member of the ESF College of Expert Reviewers, 2016-
- Selection committee member for the Hamburg Prize for Theoretical Physics 2016
- Member of the judging panel for the CECAM Berni J. Alder prize (2016)
- Reviewer for the Office of Science Early Career Research Program, Office of Basic Energy Sciences U. S. Department of Energy (SC-22.11) (2016)
- Evaluator for the 2015 Tsungming Tu Award (TTA), Ministry of Science and Technology (MOST), Taiwan
- Panel Member for the Francqui Prize, given King of Belgium (2015)
- Panel Member for the Russian Science Foundation (RSF), the Russian International Affairs Council (RIAC) (2015)
- Panel Chair of the European Research Council, ERC Starting Grant 2015 PE4 (Physical and Analytical chemical Sciences)
- Panel member of the European Research Council, ERC Starting Grant 2013 PE4 (Physical and Analytical chemical Sciences)
- Panel referee for the FNP Prize of the Polish Foundation for Science in Chemistry and Material Science (2013-)
- Panel member of the Deutsche Forschungsgemeinschaft (DFG) program "Excellence Initiative" (Physics, Mathematics, Geosciences) (2011-)
- Member of Board Meeting and Evaluation Panel of the IFW Dresden (October 2008; and 2011)
- Referee for the Academy of Finland ("Research Council for Natural Sciences and Engineering"); Academy Professor evaluation (2011-)



- Referee Fundación General CSIC (2011-)
- Referee for CEA Eurotalents program (2010-)
- Referee for the European Research Council (Starters, Consolidator and Advanced grants) (ERC) (2008-) (Physical and Analytical Sciences Panel and cross panel reviews)
- Scientific reviewer for PRACE (the Partnership for Advanced Computing in Europe) (2011-)
- Miembro del Panel de Expertos del Área de Física del Ministerio de Ciencia e Innovación para la selección de proyectos de I+D (Mayo 2009)
- Evaluador para las siguientes Agencias: i) Agencia Nacional de Evaluación y Prospectiva (ANEP), ii) UNIQUAL, iii) Agencia para la Calidad del Sistema Universitario de Castilla y León (ACSUCYL)
- ESF Pool of Reviews (European Science Foundation established a global, quality-driven pool of scientific peer reviewers across all areas of research) (2008)
- Selection Committee member for research positions in the "Centre for Computational Physics", Coimbra, Portugal (since 2007-)
- Panel member in the topic NMP-2007-1.2-2: "Equipment and methods for nanotechnology", European Commission 7th Framework Programme (2007)
- Vocal de la Comisión del Ministerio de Ciencia y Tecnología para la selección de proyectos de I+D dentro del Programa Nacional de Promoción General del Conocimiento, Área de Física. (Junio 2003)
- Referee for ACS Petroleum Research Fund, USA (2012-)
- Referee for the Austrian Science Fund (FWF) (2010-)
- Referee para el INFM italiano, programa "High Performance Computing" (Dec. 2000 y 2001)
- Referee para el programa marco de la Comunidad Europea: "Information Science and Technology Program" (Feb. May. 2001, 2003)
- Referee para el programa de apoyo a proyectos de investigación básica del "Consejo Nacional de Ciencia y Tecnología Mexicano (CONACYT 2001)" (Oct. 2001)
- Panellist/reviewer for the Materials panel of the Research Frontiers Programme 2007 of Science Foundation Ireland (SFI) (2006,2007)
- Referee for the Fundamental Onderzoek der Materie (FOM), The Netherlands, (2001,2004) and Division for Chemical Sciences (CW) of the Netherlands Organisation for Scientific Research (NWO)
- Referee para el CECAM (2001,2005).
- Referee para la National Science Foundation (NSF), USA (2001-)
- Referee para el National Research Council of Canada (NRC), and NRC - Hermann von Helmholtz-Gemeinschaft Deutscher Forschungszentren e.V. (HGF). (August 2002)
- Referee para el "ESF EUROCORES programme in self organised nano structures (SONS)" (2002)
- Referee para el programa "APART: Austrian Program for Advanced Research and Technology" of the Austrian Academy of Sciences, (2003).
- Referee for the BSF (United States-Israel Binational Science Foundation) (2005,2007,2012)
- Referee for Gordon Research Conferences, (2005-)
- Referee para el programa de apoyo a proyectos de investigación del Consejo Superior de FONDECYT, Chile (2006-)
- Referee for the German-Israeli Foundation for Scientific Research and Development (2007)

- Referee of the Seventh Framework Programme of the European Community for Research, Technological Development and Demonstration Activities (FP7) under the Topic: NMP-2007-1.2-2: "Equipment and methods for nanotechnology" (2007)
- Referee for IRCSET PostDoctoral Fellowship Scheme 2008
- Referee for the Singapore National Research Foundation "R&D that matters": Clean Energy Programme Office (CEPO) (2008)
- Referee for the ANR Francia (2008-)

**Editor:**

- Editorial Board Member of Oxford Materials Science" (2020-)
- Editorial Board Member of Springer Series in Solid State Physics (2019-)
- Editorial Board Member of Electronic Structure, IOP (June 2018-)
- Editorial Board Member of Proceedings of the National Academy of Science, PNAS (Applied Physical Sciences) (June 2017-)
- Assistant Editor NanoLetters (April 2017-)
- Miembro del Editorial Board of Scientific Reports (Nature) (2016-)
- Miembro del Editorial Board of ChemPhysChem (2015-2018)
- Editor in Chief European Physical Journal B (July 2011-March 2017)
- Miembro del "Editorial Board" of Lecture Notes in Physics, Springer (2011-)
- Miembro del Editorial Board of Physics Research International (2007-2017) (<http://www.hindawi.com/journals/phys/>)

**Revistas:**

- Con regularidad: Physical Review Letters, Nature, Nature Physics and Nature Materials, Science, Physical Review B, Journal of Chemical Physics, Chemical Physics Letters Applied Physics Letters, Journal of the American Chemical Society Physical Review A, Nano Letters
- En ocasiones: Chemical Review, Nature Communications, Physical Chemistry Chemical Physics, Journal of Physics: Condensed Matter, Journal of Physics B, Journal of Physical Chemistry, Foundations of Physics Letters, International Journal of Nanoscience, Solid State Communications, Physica Status Solidi, Synthetic Metals, Surface Science Iranian Journal of Science & Technology, Zeitschrift für Physik D (Atoms, Molecules and Clusters), Sensors and Actuators B, Polymers & Polymers Composites, Journal of Materials Research, New Journal of Physics, Nuclear Instruments and Methods B.