

Scientific Member and Director

Max Planck Institute for the Structure and Dynamics of Matter (MPSD)

Luruper Chaussee 149, 22761 Hamburg, Germany

And

Distinguish Professor: Condensed Matter Physics

Dpt. Física de Materiales, Facultad de Químicas and Centro Física de Materiales CSIC-UPV/EHU

*Edificio I+D+I Korta, Avenida de Tolosa 72
European Theoretical Spectroscopy Facility (ETSF)
Apdo. 1072, 20018 San Sebastián/Donostia. Spain*

Education

University of Valladolid, Spain Ph.D. in Physics (“Apto Cum Laude”), 1991.

University of Valladolid, Spain, Summa Cum Laude, B.S. in Physics, 1988.

Professional Experience

- Appointed Scientific Member and Director of the Max Planck Institute for the Structure and Dynamics of Matter (MPSD) in Hamburg
item Faculty member of the Wolfgang Pauli Centre, Hamburg (2015-)
- Miller Visiting Professor, University of California at Berkeley (August-September 2014)
- Full Professor Condensed Matter Physics (Chair), University of the Basque Country, Spain, April-2001-present
- *Visiting Professor (Iere class)*, Universidad de Montpellier 2, Francia, June-July 2007.
- *Visiting Professor (Humboldt)*, Freie Universitat Berlin, 2005.
- Associated to Centro Mixto CSIC-UPV/EHU and DIPC, San Sebastián, Spain, April-2001-present
- *Visiting Professor*, Department of Physics, Freie Universität Berlin, Berlin, Germany, (June-2006-July 2007)
- *Visiting Professor*, Laboratoire des Solides Irradiés, Ecole Polytechnique, Palaiseau, France. Dec.2000-Apr.2001.
- *Visiting Professor (Iberdrola)*, Dpto. Física de Materiales, Universidad del País Vasco, Donostia Apr-Sep.1998.
- *Associate Professor*, Dpt.Física Teórica, Atómica, Molecular y Nuclear, University of Valladolid, Dec.93-Apr.01
- *Fulbright Postdoctoral and Research Associate Fellow* Department of Physics, University of California at Berkeley, and Materials Sciences Division LBL, Berkeley, USA. Oct.92-Sep.94
- *Assistant Professor*, Dpt. Física Teórica, Atómica, Molecular y Nuclear, University of Valladolid, Oct.91-Oct.92
- *Research Fellow of “Ministerio de Educación y Ciencia”* Dpt. Física Teórica. Universidad de Valladolid. Spain. January 1988-October 1991 and *Research Felows “Caja de Ahorros y Monte de Piedad de Madrid*

Selected Awards and Fellowships

- JSPS Invitation Fellowship for Research in Japan, 2016
- XV Manuel Laborde Werlinden Prize for the best technology-based business initiative based on innovative ideas: “Materials Evolution”, December 2015
- Premio Jaime I de Investigación Básica 2014.
- Foreign associate member of the National Academy of Sciences (NAS) of United States (2014)
- External Scientific Member of the Fritz-Haber-Institute of the Max-Planck-Gesellschaft, (Nov. 2011-)
- European Research Council (ERC) Advanced Grant (2011-2016) (DYName)

- *"Distinguished Visiting Scientist"*, Fritz Haber Institute der Max-Planck-Gesellschaft, Berlin (2009-)
- *Outstanding Referee*, American Physical Society (2009)
- Dupont Prize in Nanotechnology, Dupont Foundation (2006)
- Friedrich Wilhelm Bessel Research Award, Humboldt Foundation (2005)
- Fellow of the American Physical Society, Division of Materials Science (2004)
- Sir Allan Sewell Fellowship, Australia, 2004
- SPS Invitation Fellowship Programs for Research in Japan, 2001
- Salvador de Madariaga Fellow, 2000-1
- Fulbright Fellow, 1992-94
- *Real Spanish Physical Society Prize "Jóvenes Investigadores"* Madrid. Spain. July, 1992
- *Honor Prize for the best Ph.D. Thesis in Physics* University of Valladolid. Spain. June, 1992.
- *1st National Prize for Graduated in Physics* October 25, 1989.
- *Honor Prize for the Master in Physics* and *Caja de Ahorros y Monte de Piedad de Salamanca Prize for the best graduate curriculum in the Faculty of Science in the 1988 academic year* University of Valladolid. Spain. 1989.

Research Interests

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.

Summary of CV

More than 300 publications in scientific journals, with more than 25000 citations in total (index h=76). Three reviews of modern physics. Editor of three books about nanotechnologies. More than 200 invited talks in international conferences/workshops.

Two **Patents**: one Field emission source with BN nanotubes, University of Valladolid, Spain P-9802690 (3-9-2001) and another on "ultraviolet optical device with bn-nanotubes" (2011).

Selected Professional and Synergetic Activities

- Selection committee member for the Hamburg Prize for Theoretical Physics 2016
- Member of the Scientific Advisory Committee of CECAM (since 2015-)
- Member of the judging panel for the CECAM Berni J. Alder prize (2016)
- Evaluator for the Office of Science Early Career Research Program, Office of Basic Energy Sciences U. S. Department of Energy (2016)
- Member of 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 European Research Council (ERC) (2015) (Physical and Analytical Sciences P4 Panel- Starting Grants)
- Member of the Editorial Board of ChemPhysChemx
- Chair of the European Theoretical Spectroscopy Facility (ETSF) (<http://www.etsf.eu>) (since 2012-); Vice-President for Scientific Development (since 2008) and member of the Steering Committee.
- Member of the "Centro de excelencia en Nanociencia Molecular ISIC-NANO", Valencia (2012-)
- 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-)
- Editor in Chief European Journal of Physics B (since July 2011-)
- Panel member of the Deutsche Forschungsgemeinschaft (DFG) program "Excellence Initiative" (Physics, Mathematics, Geosciences) (2011-)
- 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 Board Meeting and Evaluation Panel of the IFW Dresden (October 2008; and 2011)
- Referee for the European Research Council (ERC) (2008-) (Physical and Analytical Sciences Panel)
- Editorial Board on Springer Lecture Notes in Physics (2011-)
- Referee for the Academy of Finland; Academy Professor evaluation (2011-)
- Referee Fundación General CSIC (2011-)
- Referee for CEA Eurotalents program (2010-)
- Member of the Prize Committee "Psi-k Volker Heine Young Investigator Award", 12-16 September 2010, Berlin, Germany.
- Scientific reviewer for PRACE (the Partnership for Advanced Computing in Europe) (2011-)

- ESF Pool of Reviews (European Science Foundation established a global, quality-driven pool of scientific peer reviewers across all areas of research) (2008)
- Member of the expert Panel "Área de Física" of the Ministerio de Ciencia e Innovación for I+D projects (Mayo 2009)
- Referee for the national funding agencies: i) Agencia Nacional de Evaluación y Prospectiva (ANEP), ii) UNIQUAL, iii) Agencia para la Calidad del Sistema Universitario de Castilla y Len (ACSUCYL)
- Host group for the HPC++ Europe
http://www.hpc-europa.org/index.php?section=Transnational&subsection=host_departments&page=host_departments.BSC
- Member of the BIFI "Instituto de Biocomputación y física de sistemas complejos", Zaragoza, Spain (since January 2008-)
- Member of the Scientific Council of the GDR-E Nano-I on Science and Applications of Nanotubes, CNRS (France) (2007-)
- 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.cecam.org/>) MSCF-CT-2005-029252 (2006-)
- Member of the Board of Directors (Trustee) 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-)
- Advisory Board Member and Physical Scientist associated to the *ITR: Institute for the Theory of Advanced Materials in Information Technology* University of Minnesota, (Director Prof. J. Chelikowsky). Supported by the National Science Foundation (2003-)
- Spanish representative in the Steering Committee of ESF Research Networking Programmes- INTELBIOMAT ("Interdisciplinary Approaches to Functional Electronic and Biological Materials") (2008-)
- Co-cordinator of the Working group of the Spanish network on nanoscience (NANOSPAIN): Nanobiotecnología de la red NANOSPAIN" (<http://www.nanospain.org/>)
- Core-group member of the ESF programme "Towards Atomistic Materials Design" (2002-present)
- Spokesperson of the Nanostructures and nanotechnologies working group of the psi-k network (European Science Foundation Programme "Electronic Structure Calculations for Elucidating the Complex Atomistic Behaviour of Solids and Surfaces" and now "Towards Atomistic Materials Design"). Member of the International Advisory Board for the Psi-k 2000 and 2005 Conferences in Schwäbisch Gmünd, Alemania (22-26 Agosto 2000) and (17-21 September 2005); and member of the next one in 2010.
- 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 "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)
- Co-organiser of the ZCAM workshop "Databases in Quantum Chemistry", Zaragoza 22-14 September 2010.
- 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
- 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.
- Member of the Scientific Committee of Cargèse International School, Cargèse, Corsica, France 3-15 Julio 2006 and NATO ASI School on *Carbon Nanotubes: From Basic Research to Nanotechnology* Sozopol, Bulgaria 21-31 May (2005).
- "Programm Committee" of *International Winterschool on Electronic Properties of Novel Materials Molecular Nanostructures (IWEPMN)* (2003-to date) Marzo, Kirchberg/Tirol, Austria
- 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); January 2-15 (2010)
- Co-director of the SANES workshop "Integrated Self-Adjusting Nano-Electronic Sensors" San Sebastián, 26-27 February 2009
- 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)
- Vice-chair of the Gordon conference "Time-Dependent Density-Functional Theory", Colby College Waterville, ME, USA, July 15-20, 2007
- Advisory Editorial Board of *Journal of Nanoscience and Nanotechnology* (2001-2003); "Editorial Board" of the *International Journal of Materials Science and Semiconductors*, (2006-); and of *Physics Research International* (2007-) (<http://www.hindawi.com/journals/phys/>)
- Advisor to "Information Science and Technology Program" of the European Union (2000-present)
- Chair and organising committee member to numerous international conferences/workshops: APS, MRS in USA and EPS, ESF, CECAM in Europe.
- Referee for the following financial agencies: Spanish Ministry of Science and Education and member of the panel evaluating projects in Physics; National Science Foundation (NSF), USA (2001-present); European Commission (2000-present), European Science Foundation (2002-present); Fundamental Onderzoek der Materie (FOM), The Netherlands, (Nov. 2001); Council for Chemical Sciences (CW) of the Netherlands Consejo Nacional de Ciencia y Tecnología Mexicano (CONACYT 2001)" (Oct. 2001); INFN italiano (Dec. 2000 y 2001), National Research Council of Canada (NRC), and NRC - Hermann von Helmholtz-Gemeinschaft Deutscher Forschungszentren e.V. (HGF) (2002), Austrian Academy of Sciences (2003); Council for Chemical Sciences (CW) of the Netherlands (NWO) (2005); The Research Council of Norway, Division of Science (2005); BSF (United States-Israel Binational Science Foundation) (2005); Agence National de la Recherche (ANR), France (2005-); Gordon Research Conferences, (2005-) Research Frontiers Programme 2007 of Science Foundation

Ireland (SFI) (2006), Consejos Superiores de FONDECYT Chile (2006); Selection Committee member for research positions in the "Centre for Computational Physics", Coimbra, Portugal (2007-)
Referee for permanent research positions at the CNRS in France, and CSIC in Spain.

Research projects (in the last 10 years)

1. *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.
2. *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.
3. *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.
4. *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.
5. *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
6. *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**
7. *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 €
8. *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
9. *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**)
10. *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**
11. *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**
12. *Spectroscopic properties of biomolecules, nanostructures and extended systems (ETSF activity)*
Proyectos del Centro Nacional de Supercomputación (Mare Nostrum), FI-2006-3-0007; FI-2006-4-0017; FI-2007-1-0011; FI-2007-2-0012; FI-2007-3-0024
Investigador Principal: **Angel Rubio**

13. *Optical Properties of BN Nanotubes and Hexagonal BN (ETSF activity)*
Proyectos de la Red Española de Supercomputación, FI-2009-1-0006; FI-2008-3-0014; FI-2008-2-0035
Investigador Principal: **Angel Rubio**
14. *Optical and Charge Transfer Properties of Hybrid Organic-Dye/Oxide Nanostructure and Interface Systems for Solar Cells Application (ETSF activity)*
Proyectos de la Red Española de Supercomputación, FI-2009-2-0026, FI-2009-3-0009, FI-2010-1-0002, FI-2010-2-0020
Investigador Principal: **Angel Rubio**
15. *Towards understanding strong electronic correlation in transition-metal oxides from first principles: a theoretical spectroscopy approach*
Proyectos de la Red Española de Supercomputación, FI-2010-3-0001
Investigador Principal: Matteo Gatti and **Angel Rubio**
16. *Characterization of the optical absorption spectrum of Cationic porphyrins stacked in DNA derivatives by means of Time Dependent Density Functional Theory*
Proyectos de la Red Española de Supercomputación, QCM-2010-3-0012
Investigador Principal: Daniele Varsano and **Angel Rubio**
17. *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)
18. *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**
19. *Etude des propriéts physiques des nanomatériaux base de carbone*
Agencia Española de Cooperación Internacional AECI PCI-Mediterráneo (A/9817/07) (2008) Dotación: 4500 €
Investigador Principal: **Angel Rubio**
(en colaboración con Faculte des sciences (Mknes) Prof. Abdelali Rahmani)
20. *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**.
21. *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**
22. *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**
23. *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**
24. *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**

25. *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€).
26. *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.
27. *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**)
28. *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**
29. *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**
30. *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 (1/1/11-31/12/2013) (FIS2010-21282-C02-01) Dotación: 176.500 €
Investigador Principal y Coordinador del Proyecto global: **Angel Rubio**
31. *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
32. *Tailoring Electronic and Phononic Properties of Nanomaterials: Towards Improved Thermoelectricity (nanoTHERM)*
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
33. *Dynamical processes in open quantum systems: pushing the frontiers of theoretical spectroscopy (DYName)*
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**
34. *Computer simulations of thermally excited molecules and materials by first principles (TEMMIP)*
International Research Staff Exchange Scheme (FP7-PEOPLE-2011-IRSES)(grant 295172) cuatro años (2012-2015)
Coordinator: Dr. T. Heine (Jakobs University, Germany)
Co-ordinator in Spain: **Jesus Ugalde and Angel Rubio**
35. *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: 243280 €
Coordinator: Dr. S. Sanvito (Trinity College, Dublin)
Co-ordinator in Spain: **Angel Rubio**

36. *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**
37. 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 €
38. 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 Lebedeva (2013-2015) Host in Spain: **Angel Rubio** 166,336.20 €
39. *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**
40. *COST ACTION MP1306 "Materials, Physical and Nanosciences"*, Chair: H. Ebber, Member of the Management Committee: **A. Rubio** (2014-2016)
41. *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 (1-12-2014;31-12-2016) (FIS2013-46159-C3-1-P) Dotación: 129.470,00 €
 Investigador Principal y Coordinador del Proyecto global: **Angel Rubio**
42. *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 110000 \$ (Feb-2015-2018)
 Principal Investigator in Spain **Angel Rubio**
43. *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 €
44. *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 €
45. *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**
46. *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**
47. *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**

48. *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) Germnay: **Angel Rubio** 159640,80 €
49. *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 €
50. *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 €
51. *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 €
52. *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 €

Invited Talks in the last 10 years

1. *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
2. *Excited state dynamics of nanostructures and biomolecules within TDDFT*
Spring meeting of the DPG, Frankfurt, Alemania 17-Marzo-2006
3. *Weak interactions in layered materials within the ACDFD framework*
van der Waals Workshop (vdW²) on Weak Chemical and Physical Interactions, 6-7 June 2006 SISSA, Trieste, Italy 7-June-2006
4. *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
5. *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
6. *Boron nitride nanotubes*
CAPE Advanced Technology Lectures and Seminars, Cambridge, UK 15-Diciembre-2006
7. *Spectroscopic Properties of hexagonal Boron Nitride and Nanotubes*
International Winterschool on Electronic Properties of Novel Materials (IWEPM2007), March 10-17 (2007), Kirchberg/Tirol, Austria 15-Marzo-2007
8. *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
9. *BN nanotubes*
CNR-INFN National Research Center S3 (nanoStructures and bioSystems at Surfaces) Modena, Italy 11-April-2007
10. *Theoretical description of the spectroscopic properties of biomolecules and nanostructures*
Coloquio, Instituto de Ciencia Molecular (ICMol) Universidad de Valencia 24-Abril-2007
11. *Excited state properties of biomolecules: a TDDFT study* Coloquio del Institute for Biocomputation and Physics of Complex Systems, BIFI, Zaragoza, 11-Mayo-2007
12. *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
13. *Structural dynamics in the excite state within a tddft formalims*
International Workshop on "Non-Adiabatic Dynamics at Surfaces" Schloss Reizensburg, Germany, 22-25. October 2007 24-October-2007
14. *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
15. *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
16. *Dimensionality effects in the optics of BN nanostructures: role of defects*
Nanospain 2008, Braga, Portugal 14-19 Abril 2008 16-Abril-2008
17. *Modelling the response to external stimulus of biomolecules*
Biophysics Colloquium of the Center for Computational Physics Coimbra, Portugal 16-Abril-2008

18. *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
19. *Carbon nanotubes for renewable energy*
Journée NAno EnR'08, Universite Montpellier 2, France 4-June-2008
20. *Nanociencia: conceptos y aplicaciones*
Garrigues Donostia 16-Junio-2008
21. *Optical Properties of BN nanostructures: role of Defects and dimensionality effects*
NT08 (CCTN08 symposium) Montpellier Francia, 28 Junio-4 Julio (2008) 28-Junio-2008
22. *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
23. *The world of nanotubes: new properties and applications*
II workshop en Nanociencia y Nanotecnología Analíticas. Tarragona, 25-26 Septiembre 2008 25-Septiembre-2008
24. *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
25. *Excited state dynamics of nanostructures and biomolecules within time-dependent DFT*
Institute of Solid State and Materials IFW Dresden, Germany 22-January-2009
26. *What is the European Theoretical Spectroscopy Facility (ETSF) : the emergence of a new infrastructure*
NFFA (Nanoscience Foundries and Fine Analysis) meeting, Centro Nacional de Microelectronica (CSIC) Campus UAB, Spain 2-March-2009
27. *Boron Nitride and graphene nanostructures: properties and applications*
NanoCenter Seminar, Pittsburgh, USA 17-March-2009
28. *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
29. *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
30. *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
31. *Theoretical spectroscopy of nanostructures and biomolecules*
Colloquio of Institut fr Physikalische Chemie Universitt Würzburg, Germany 2-June-2009
32. *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
33. *Theoretical Spectroscopy of Complex Nanostructures and Biomolecules*
XXIV International Conference on Photochemistry ICP2009, 19-24 July 2009 Toledo Spain 22-July-2009
34. *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
35. *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

36. *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
37. *Boron Nitride and Carbon nanotubes*
International Conference on Carbon Nanostructured Materials
Santorini, Greece 4 - 8 October 2009 6-October-2009
38. *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
39. *Efficient implementation of time-dependent density functional theory for biomolecules and nanostructures*
Department of Mathematics, UC Santa Barbara, 9-NOVIEMBRE-2009
40. *Theoretical spectroscopy of low dimensional systems*
Center for Excitonics, Cambridge, MIT, Harvard 11-NOVIEMBRE-2009
41. *Spectroscopy of complex nanostructures and biomolecules*
SISSA & DEMOCRITOS National Simulation Center, Trieste, Italy 8-Abril-2010
42. *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
43. *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
44. *Simulation the excite state dynamics of complex nanostructures and biocomplexes*
Colloquium of the Max-Planck-Institut fuer Festkoerperforschung, Stuttgart 15-June-2010
45. *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
46. *Nanostructured materials: New charge transfer solids and optoelectronic devices*
Abschieds-Kolloquium, FU Berlin, Fachbereich Physik, Berlin 1-July-2010
47. *Excited state dynamics of low-dimensional systems and biomolecules*
FHI, Department of Physical Chemistry, Berlin 5-July-2010
48. *Efficient Formalism for Large Scale Ab Initio Molecular Dynamics and mixed quantum classical dynamics with the correct equilibrium distribution*
 Ψ_k Conference 2010, 12-16 September 2010, Berlin 14-September-2010
49. *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
50. *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
51. *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
52. *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
53. *Ab-initio modeling of nanostructured-based devices for optoelectronic applications*
Colloquium Fakultät für Physik, Universität Wien, Austria 14-March-2011

54. *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
55. *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
56. *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
57. *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
58. *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
59. *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
60. *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
61. *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
62. *Boron Nitride and graphene nanostructures: properties and optoelectronic applications*
Columbia University (Depts of Physics and Electrical Engineering) 15-August-2011
63. *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
64. *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 Systeme, Dresden 27-September-2011
65. *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
66. *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
67. *Modeling Nanostructured materials*
Coloquium Institute of Solid State and Materials IFW Dresden, Germany, 10th November 2011
68. *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
69. *Modeling optoelectronic nanostructured devices made of inorganic nanotubes*
Colloquium Physics Department of the University Duisburg-Essen, Germany 14-December-2011

70. *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
71. *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
72. *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
73. *TDDFT for light-matter interactions in strong coupling regimes*
2nd TYC workshop on energy materials, 6-8 June 2012, London, UK 7-June-2012
74. *Simulating optoelectronic devices at the nanoscale: a TDDFT perspective*
2nd International Conference on Advanced Materials Modelling (ICAMM), Institut des Matériaux Jean Rouxel, June 13-16, Nantes France 14-June-2012
75. *Unraveling the electronic properties of nanostructures and biomolecules from spectroscopy: a theoretical perspective*
Concepts and Applications of Stimulus-responsive Materials
Summer UPV/EHU Workshop, Donostia June 20-22 (2012) 21-June-2012
76. *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
77. *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
78. *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
79. *What time-dependent density functional theory can provide to understand and design nanostructured-based optoelectronic materials*
Colloquium Department of Chemistry, Technische Universität München, Garching 18-October-2012
80. *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
81. *Predicting properties of nanostructures and biomolecules*
Public Lecture, University of Luxembourg, 12th-November-2012
82. *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
83. *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 So Paulo 12 December 2012
84. *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
85. *New nanoscale hybrid structures made of C and BN from first principles: optoelectronic devices*
International Winterschool on Electronic Properties of Novel Materials (IWEPM2013), March 2-9 (2013), Kirchberg/Tirol, Austria 4-March-2013

86. *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
87. *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
88. *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
89. *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 3-July-2013
90. *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
91. *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
92. *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
93. *Impacto de la teora en Nanociencia: nuevos materiales y dispositivos*
Nanotecnología, Fundación Valenciana de Estudios Avanzados, Valencia 15-November-2013
94. *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 Novem-
ber 2013 22nd-November-2013
95. *Open session about challenges and standing problems*
6th Time-Dependent Density-Functional Theory: Prospects and Applications, Benasque, 4-18 January 2014
13-January-2014
96. *Light-induced processes in finite and extended systems from TDDFT*
VI International Conference of the Institute for Biocomputation and Physics of Complex Systems (BIFI), "Ex-
ploring the role of computation in Science: from Biology to physics", Zaragoza (Spain), January, 22-24, 2014.
22-February-2014
97. *Non equilibrium dynamical processes in low dimensional systems from a time-dependent density functional perspective*
Colloquium of the Institut fr Physikalische Chemie Universitt Würzburg, Germany 11-February-2014
98. *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
99. *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
100. *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
101. *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
102. *Modeling optoelectronic and hybrid-photovoltaic devices within TDDFT*
Colloquium Physikalische Chemie, Department of Chemistry, Universität München 4th-June-2014

103. *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
104. *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
105. *Optoelectronic and hybrid-photovoltaic devices from first principles simulations*
Seminar of the Physical Chemistry department (ISIC) at the EPFL, Lausanne 12-July-2014
106. *Ab initio modelling of light-induced non equilibrium dynamical processes in organic materials*
Department of Physics, Stanford University, USA 22-August-2014
107. *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
108. *First principles modeling of photovoltaic and optoelectronic devices: fundamentals and applications*
Department of Chemistry, University of California, Berkeley, USA 12-September-2014
109. *Modeling non equilibrium dynamical processes in TDDFT: optoelectronic and photovoltaic applications*
Physical Seminar, University of Rochester, USA 15-September-2014
110. *Non equilibrium dynamical processes in TDDFT: organic photovoltaic applications*
Colloquium Molecular Foundry, Lawrence Berkeley Laboratory, Berkeley 16-September-2014
111. *Theoretical Spectroscopy: TDDFT*
7th European School on Molecular Nanoscience (ESMOLNA2012), Gandia (Spain), 26th to 30th October 2014
27th-October-2014
112. *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
113. *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
114. *Novel electronic and structural properties of two-dimensional materials:silicene, germanene and stanene*
Emerging Non-Graphene 2D Atomic Layers and van der Walls Solids.Symposium of the Fall Materials Research Society (MRS) meeting, Boston 3-December-2014
115. *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
116. *Simulation of photon-matter interactions within QED-TDDFT*
SWOCS V, Symposium of Computational Science, POSCO International Center, Pohang, Korea 3-February-2015
117. *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
118. *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
119. *Extending time-dependent density functional theory to account for treating 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-October-2015

120. *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
121. *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
122. *Group IV two-dimensional materials : Novel electronic and structural properties*
Colloquium Institute of Solid State and Materials IFW Dresden, Germany, 24th November 2015
123. *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
124. *A TDDFT formulation for strong light matter interactions : applications to energy conversion*
Coloquium Institut fuer Theoretische Physik, Technische Universitaet Dresden, Dresden, Germany, 26-January-2016
125. *First principles modeling of light-induced ultrafast phenomena in nanostructures and solid*
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
126. *Strong light-matter interactions and quantum entanglement: merging QED and TDDFT*
Colloquium Department of Physics, University fo Pennsylvania 16-February-2016
127. *Quantum Electrodynamical Density Functional Theory: light-matter interactions and entanglement*
Ultra-fast phenomena in quantum physics: a challenge for theory & experiment, CECAM-HQ-EPFL, Lausanne, Switzerland, April 11-15, 2016 12-April-2016
128. *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

Teaching

Undergraduate teaching experience (summary)

At the University of Valladolid: Atomic and Molecular Physics, Mathematical Methods, Computing, Quantum Mechanics, Advanced Quantum Mechanics, Nuclear Physics, Relativistic Theory.

At Berkeley University: Thermal Physics

At the University of the Basque Country: Solid State Physics, Basic Concepts in Solids: Fundamentals and applications, professor in the doctorate program of excellence by the Ministry of science and Education: "PHYSICS OF NANOSTRUCTURES AND ADVANCED MATERIALS (Master in Nanoscience)". 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/>

Graduate Courses

- Profesor del programa de Doctorado con mención de calidad del MEC: "PHYSICS OF NANOSTRUCTURES AND ADVANCED MATERIALS (Master in Nanoscience)" (since 2007-)
Master courses:
Excited-state properties of low-dimensional systems
Low dimensional systems and nanostructures
Nanostructural properties
- Professor of the "Leibniz graduate school DinL: Dynamics in new Light" (2010-)
- Professor of the "master inter-universitario en Nanociencia y Nanotecnología Molecular, coordinado por el Prof. Eugenio Coronado, Universidad de Valencia"(2007-)
- 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 sobre "Time-Dependent Density-Functional-Theory and its Applications"
Departamento de Física de Materiales, Universidad del País Vasco, San Sebastian. (30-Junio al 4-Julio 1997)
- Spring College on "Electronic Structure Approaches to the Physics of Materials". International Centre for Theoretical Physics (ICTP), Trieste, Italia (15 May - 9 June 2000)
- "III Taller de Física Computacional: Aplicaciones de los Metodos Ab-Initio en Materia Condensada". Merida, Venezuela (10 al 14 de Julio del 2000)
- "Nuevas estructuras moleculares, los nanotubos: estructuras, propiedades y aplicaciones en nanotecnología"
VI Escuela Nacional de Materiales Moleculares, Cartagena, Murcia (21-29 Junio 2003)
- Spring College on "Science at the Nanoscale"
International Centre for Theoretical Physics (ICTP), Trieste, Italia (24-31 May 2004)
- 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)
- School on "Time-Dependent Density-Functional Theory: Prospects and Applications",
Benasque Center for Science, Benasque, Huesca (Spain) August 29-September 11, (2004)
- 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)
- 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 electronica de sistemas moleculares: espectroscopía y transporte en nano-estructuras y biomoléculas)

Master Thesis

- *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*
Kaiké 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 Khaledi, 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, 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, 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, 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^a. Begoña Torres Cabrera (Julio 1993) Calificación : Sobresaliente con Honor.
Codirigida con el Prof. Luis Carlos Balbás Ruesgas.

PhD Thesis

1. *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
2. *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, July 2013, Director M. Scheffler, Co-director: . Rubio
3. *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, July 2013, Director M. Scheffler, Co-director: . Rubio
4. *Theoretical Description of the Optical Properties of Nanostructures Within Time Dependent Density Functional Theory*, Leonardo Andrés Espinosa Leal, European PhD Thesis Directed by Ángel Rubio and Daniele Varsano,
5. *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
6. *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
7. *Improving simulation of biological molecules: refining mathematical, physical and computational tools*, Pablo García Risueño, 15th December 2011, European Thesis Directed by José Luis Alonso, Pablo Echenique and Ángel Rubio
Sobresaliente Cum Laude
8. *Linear and non-linear response phenomena of molecular systems within time-dependent density functional theory*. Xavier Andrade, 8th October 2010. European Thesis directed by Angel Rubio and Silvana Botti
Sobresaliente Cum Laude
9. *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
10. *First principles description of response functions in low dimensional systems* . Daniele Varsano. 13-Julio-2006.
Sobresaliente Cum Laude.

11. *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)
12. *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)
13. *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)
14. *Resonancia Magnética Nuclear en Nanotubos de Carbono* Sylvain Latil. (Septiembre 2001) (codirigida con el Dr. Patrick Bernier de la Universidad de Montpellier)

Supervision of postdocs, sabbatical and permanent staff

1. Dr. Florian Eich, Marie Curie Intra European Fellowship (IEF) (Oct-2016-); Postdoctoral fellow MPSD (Oct-2015-Sept-2016)
2. Dr. Cesar A. Rodriguez-Rosario, Marie Curie Intra European Fellowship (IEF) (April-2016-)
3. Dr. Juan Borje, Marie Curie Intra European Fellowship (IEF) (May-2016-); Postdoctoral Fellow (March-2015-April-2016)
4. Dr. Ali Abedi, Marie Curie Intra European Fellowship (IEF) (May-2016-); Postdoctoral Fellow (Jan-2015-April-2016)
5. Dr. Elham Khosravi, Marie Curie Intra European Fellowship (IEF) (May-2016-); Postdoctoral Fellow (Jan-2015-April-2016)
6. Dr. Nicolas Tancogne-Dejean, Contrato postdoctoral MPSD (Jan-2016-)
7. Dr. Henning Glawe, Contrato postdoctoral-NOMAD MPSD (Nov-2015-)
8. Dr. Soren Nielsen, Contrato postdoctoral MPSD (Nov-2015-)
9. Dr. Iris Theophilou, Contrato postdoctoral MPSD (Oct-2015-)
10. Dr. Arun Debnath, Contrato postdoctoral MPSD (Sep-2015-)
11. Dr. Thomas Brumme, Contrato postdoctoral MPSD (Sep-2015-)
12. Dr. Michael Ruggenthaler, Contrato postdoctoral MPSD (Sep-2015-)
13. Dr. Adriel Dominguez, Contrato postdoctoral MPSD (Jun-2015-)
14. Dr. Michael Sentef, Contrato postdoctoral MPSD (Apr-2015-)
15. Dr. Andrea Droghetti, Contrato Juan de la Cierva (octubre 2014-)
16. Dr. Philipp Wopperer, Contrato Postdoctoral (Junio-2014-)
17. Dr. Hannes Huebner, Marie Curie Intra European Fellowship (IEF) (Oct-2014-)
18. Dr. Heiko Appel, Contrato postdoctoral MPSD (March-2015-); FHI-postdoc (2010-2015)
19. Dr. Stefan Kurth, Profesor Ikerbasque, (Octubre 2008 -)
20. Dr. Ilya Tokatly, Profesor Ikerbasque, (Diciembre 2007-)
21. Dr. Roberto D'Agosta, Contratado Postdoctoral del Proyecto FANCYNANO (19-Noviembre-2008;31-Marzo-2009); Profesor Ikerbasque (Abril 2009-)
22. Dr. Ravindra Laxman Shinde, Contrato Postdoctoral (Setp-2014-Oct-2015)
23. Dr. Sener Sen, Contrato Postdoctoral (5-May-2014-)

24. Dr. Lede Xian, Contrato Postdoctoral (Jan-2014-)
25. Dr. Joaquim Sornet Somoza, Beatriu de Pinós fellowship, Montpellier-Donostia (December 2012-2014); Juna de la Cierva (iOct. 2015-)
26. Dr. Seymour Cahangirov, JAE-doc CSIC (Sep-2012-March 2013); Marie Curie (April 2014-Aug-2015)
27. Dr. Ask Hjorth Larsen, Contrato Postdoctoral (March-2012-)
28. Dr. Alejandro Pérez Paz, Contratado Postdoctoral (Oct-2010-)
29. Dr. Umberto de Giovannini, Contratado Postdoctoral UPV/EHU (2010-)
30. Dr. Irina Lebedeba, Contratado Postdoctoral DYNAPLEX (Oct-2012-June-2013); Maria Curie Actions-International Incoming Fellowships (IIF) (FP7-PEOPLE-2012-IIF, Project: 326435) (June-2013-May-2015)
31. Dr. Guillermo Albareda, Beatriu de Pins fellowship FHI-Berlin (April 2012-2014)
32. Dr. Victor Morón Tejero, Contratado Postdoctoral UPV/EHU (Oct-2012-)
33. Dr. David Cardamone, Contrato Postdoctoral (Oct-2011-Dec-2014)
34. Dr. Duncan Mowbray, DIPC Postdoc (15-Septiembre-2009-Abril-2011); Juan de la Cierva (April-2011-March 2014); GV Postdoc (April-Dec 2014)
35. Dr. Marius Wanko, Consolider postoc (2009-2010); Juan de la Cierva (January-2011-Dec.-2013); GV Postdoc (Jan-2014-)
36. Dr. Yann Pouillon, Becario Postdoctoral del Programa Europeo IST, SANES (Sep.-2006, Dic.2008), Técnico doctor (2009-)
37. Dr. Amilcare Iacomino, JAE-doc CSIC (May 2010,-Nov. 2013)
38. Dr. Daniel Rohr Marie Curie Actions-Intra-European Fellowships (IEF) (FP7-PEOPLE-2011-IEF, Project: 302603) (April-2013-March-2015)
39. Dr. Ermin Malic Fritz-Haber-Institut Max-Planck-Gesellschaft, Berlin (Germany) (Jan-2013-Apr-2013)
40. Dr. Elena Cannuccia, Contratado Postdoctoral (June-2011-January 2013)
41. Dr. Annapaola Migani. JAE-doc CSIC (Sep-2010-Dic.-2012)
42. Dr. Lorenzo Stella, Contratado Postdoctoral UPV/EHU (Sep-2010-Jan.2013)
43. Dr. Matteo Gatti, Contratado Juan de la Cierva, Enero 2009-2011, Postdoc Grupos Consolidados (2012).
44. Dr. Federico Iori, Contratado Postdoctoral (Sep-2010-Apr-2011); Postdoc UPV/EHU (May 2011- Nov. 2011)
45. Dr. Jose Luis Cabellos Quiroz, Postdoc del Gobierno Mexicano (Dec-2010-Dec-2011)
46. Dr. Claudio Attaccalite, Contratado Juan de la Cierva, Diciembre 2007-2010
47. Dr. Juan Maria Garcia-Lastra, Contratado Juan de la Cierva, Dic. 2006-2009; Contratado Postdoctoral del Proyecto Europeo THEMA-CNT (Dic.-2009-Dic.2010)
48. Dr. Pierluigi Cudazzo, Contratado Postdoctoral del Proyecto FANCYNANO (1-Junio-2009-August 2014) y ERA-CHEMISTRY (10-Febrero-2009;30-Mayo-2009)
49. Dr. Letizia Chiodo Contratada Postdoctoral del Proyecto Europeo NANO-ERA Chemistry(15-June;Octubre-2008) y Postdoc UPV/EHU (1-Septiembre-2008-31-Enero-2010)
50. Dr. Nicole Helbig, Contrato Postdoctoral asociado a NANOQUANTA/ETSF, Noviembre-2007,Diciembre 2010.
51. Dr. Matthieu Verstreatte, Contratado Postdoctoral del Proyecto Europeo NANO-ERA Chemistry (May-2008; Agosto 2009)
52. Dr. Kristian Sommer Thygesen, Becario Postdoctoral del Programa Europeo IST, SANES (Sept-2005, Sept-2006)

53. Dr. Michel Bockstedte, DFG-postdoctoral fellowship (Abril-2005, Diciembre 2006)
54. Dr. Francesco Sottile, Becario Postdoctoral de la Red de Excelencia NANOQUANTA (Nov-2004, Apr-2006)
55. Dr. Mathieu Dubois, Beca Postdoctoral, (Enero-Febrero 2005)
56. Dr. Myrta Gruening: Contrato Postdoctoral del DIPC (Noviembre-2003-Diciembre 2005)
57. Dr. Ludger Wirtz: Contrato Postdoctoral del Programa Europeo RTN, COMELCAN (Febrero-2002,Diciembre-2004)
58. Dr. Andrea Marini: Contrato Postdoctoral del Programa Europeo RTN, NANOPHASE (Junio-2002,Junio-2004)
59. Dr. François Triozon: Becario Postdoctoral del Programa Europeo RTN, COMELCAN (Septiembre-2002,Febrero-2003)
60. Dr. Miguel Marques: Contrato Postdoctoral del Programa Europeo RTN, NANOPHASE (Junio-2000,Diciembre-2002)
61. Dr. Franck Rabilloud: Contrato Postdoctoral del Programa Europeo RTN, COMELCAN (Enero-2001,Octubre-2001)
62. Dr. Stephan Roche: Contrato Postdoctoral del Programa Europeo TMR, NAMITECH (Agosto-1999,Septiembre-2000)
63. Dr. Juan Arellano, Universidad de Valladolid (1999-2000)
64. Dr. Eduardo Hernández: Contrato Postdoctoral del Programa Europeo TMR, NAMITECH (Febrero-1997,Enero-1999).
65. Dr. Christophe Goze. Estancia de Doctores Comunitarios en España dentro del Programa Europeo TMR, NAMITECH (Julio-Agosto 1997)
66. 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).
67. Oleg Gritsenko, Cátedra BBVA (1998)
68. José M. Cabrera Trujillo, Universidad de Valladolid (1994-1995).

Supervision of predoctoral students

1. Gabriel Topp, PhD Student (MPSD-Hamburg) (1-12-2015;-)
2. Fabio Covito, PhD Student (MPSD-Hamburg) (1-11-2015;-)
3. Raison Dzousa, PhD Student (MPSD-Hamburg, IMPRS) (15-9-2015;-)
4. Kyung-Min Lee, PhD Student (MPSD-Hamburg, IMPRS) (27-8-2015;-)
5. Christian Schaefer, Master Student (MPSD-Hamburg) (1-11-2014;-)
6. Nora Hoffmann, Master Student, (MPSD-Hamburg) (1-1-2015;-)
7. Florian Buchholz, Master Student, (MPSD-Hamburg) (4-1-2015;-)
8. Jean-Pierre Inchaustegui, Master Student, (MPSD-Hamburg) (9-2-2015;-)
9. Uliana Mordovina, Master Student, (MPSD-Hamburg) (1-11-2014;-)
10. Teresa Reinhard, PhD Student, (MPSD-Hamburg, IMPRS) (1-12-2014;-)
11. Tanja Dimitrov, PhD Student (FHI + MPSD) (2011-)
12. Johannes Flick, PhD Student (FHI + MPSD) (2011-)

13. René Jëstadt, Becario ERC (1-Ago-2013-May-2014); FHI-Fellowship (June 2014-)
14. Livia Noemi Glanzmann, Marie Curie Fellowship (ITN-POCAONTAS) (20-May-2013-)
15. Alejandro Varas, Becario ERC-DYNamo (15-Feb-2013-)
16. Camila Pellegrini, Becaria ERC-DYNamo, (26-Nov-2012-)
17. Robert Biele (2011-), becario Consolider NanoTherm (2011-)
18. Kaike Yang, becario Consolider NanoTherm (2011-)
19. Bruno Torcal Embeita, becario FPI (Dynaplex) (oct-2011-)
20. Mehdi Farzanehpour, becario UPV (2011-)
21. Alison Crawford Uranga, becaria GV (2010-)
22. Jessica Walkenhorst, becaria UPV (2010-)
23. Joseba Alberdi, becario UPV/EHU (2010-)
24. Fulvio Berardi, becario CSIC (2009-)
25. Martin Madel, Becario ERC-DYNamo, (26-Nov-2012-5-May-2014)
26. Marco Casadei, FHI-fellow (Jan-2009-Apr. 2014)
27. Fabio Caruso, FHI-fellow (Jan-2009-Dec-2013)
28. Johanna Fuks, Becaria asociada al proyecto FANCYNANO del MEC (3-Noviembre-2008-Junio 2013)
29. Peizhe Tang, Tsinghua University, Beijing P.R.China (Oct-2012-Apr-2013)
30. Paul Giraud Universit de Lille, France (April-September 2012)
31. Leonardo Andres Espinosa Leal, Becario asociado al Proyecto Europeo NANO-ERA Chemistry; (Octubre 2007-Junio 2008); CSIC fellow (July-2008-Dec-2012)
32. Ali Akbari, Becario asociado al Proyecto Europeo DNA-NANODEVICES y NANO-ERA Chemistry; (Agosto 2006-Junio-2008); CSIC Fellow (July 2008-Dec-2012)
33. 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)
34. Micael Oliveira, Becario del Gobierno Portugues (2003-2008), Tesis cotutelada con el Profesor Fernando Nogueira de la Universidad de Coimbra, Portugal.
35. Sebastien Le Roy, Stage from Ecole Polytechnique, France (May-July 2006)
36. Daniele Varsano, Becario de la Comunidad Europea asociado al Proyecto COMELCAN (2001-2003), y NANOQUANTA (2004-2005)
37. 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)
38. Alberto Castro, Beca de Colaboración de la Universidad de Valladolid (1999); Becario Predoctoral del Subprograma de Formación de Profesorado Universitario del MEC (2000-2004).
39. Sylvain Latil, Becario asociado al Proyecto NAMITECH, Universidad de Montpellier (1999-2001)
40. Jorge Serrano Gutiérrez, Beca de Colaboración MEC (1998); Becario Predoctoral del Subprograma de Formación de Profesorado Universitario del MEC (1999-2001).
41. Teodófilo del Caño González, Beca de Colaboración de la Universidad de Valladolid (1998); Beca de Colaboración MEC (1999).

Memberships

U.S. National Academy of Sciences, American Physical Society (APS), American Chemical Society (ACS), American Association for the Advancement of Science (AAAS), European Physical Society (EPS), Royal Spanish Physical Society (RSEF), Alexander von Humboldt Network (AvH)