

Full Professor of Condensed Matter Physics

Nano Bio Spectroscopy Group,
Dpt. Física de Materiales, Facultad de Químicas and
Centro Física de Materiales CSIC-UPV/EHU

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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

- 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

- *“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 related to the project are on: 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
- Theoretical Spectroscopy: photoemission, time-resolved and optical and magnetic spectroscopies, Raman, IR, etc.
- Nanostructures
- Biotechnology and hybrid materials: photovoltaic applications
- Molecular electronics;
- Code development

The research is supported at present by different European Research Networks and projects and by the Spanish and Basque research agencies. We also got awarded with the Vicepresidency for Scientific DEvelopment of the "European Theoretical Spectroscopy Facility (ETSF)" under an e-I3 project of the EU in the 7th Framework Program (2008-2011).

Summary of CV

More than 200 publications in scientific journals, with more than 9900 citations in total (index $h=50$). Two reviews of modern physics. ISI Essential Science Indicators in Physics, Chemistry and Materials Science (<http://isiknowledge.com>) Editor of two books about nanotechnologies. More than 90 invited talks in international conferences/workshops. One **Patent** on Field emission source with BN nanotubes, University of Valladolid, Spain P-9802690 (3-9-2001). I am vice-president for scientific development of the ETFS and advisory board member of different institutes in Europe and USA as well as panel member of many EU-funding agencies.

Selected Professional and Synergetic Activities

- Vice-President for Scientific Development of the European Theoretical Sepctroscopy Facility (ETSF) (<http://www.etsf.eu>) (since 2008) and member of the Steering Committee.
- Referee for the European Research Council (ERC) (2008-) (Physical and Analytical Sciences Panel)
- ESF Pool of Reviews (European Science Foundation established a global, quality-driven pool of scientific peer reviewers across all areas of research) (2008)
- 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.cecarn.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-coordinator 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 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
 - Chair of the Gordon Research Conference Time-Dependent Density Functional Theory, New Hampshire, USA, 5-10/07 2009
 - 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)
 - 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) and 'Editorial Board' of the *International Journal of Materials Science and Semiconductors*, (2006-)
 - 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.

Most cited articles (above 100 citations)

1. A. Rubio J.L. Corkill y M.L. Cohen,
Physical Review (Rap. Comm.) B **49**, 5081-5084 (1994) 496 citas
2. E. Hernández, C. Goze, P. Bernier y A. Rubio,
Physical Review Letters **80**, 4502 (1998) 482 citas
3. X. Blase, A. Rubio, S. G. Louie y M. L. Cohen,
Europhysics Letters **28**, 335-340 (1994) 474 citas
4. P.M. Ajayan, L.S. Schadler, C. Giannaris y A. Rubio
Advanced Materials **12**, 750-753 (2000) 470 citas
5. G. Onida, L. Reining y A. Rubio
Reviews of Modern Physics **74** 601-659 (2002) 431 citas
6. D. Sánchez-Portal, E. Artacho, J.M. Soler, A. Rubio y P. Ordejón
Physical Review B **59**, 12678-12688 (1999). 365 citas
7. A. Rubio, J.L. Corkill, M.L. Cohen, E.L. Shirley y S.G. Louie
Physical Review B **48**, 11810-11816 (1993) 255 citas
8. 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, Physical Review (Rap. Comm.) B **51**, 11229 (1995) 222 citas
9. P.J. Britto, K.S.V. Santhanam, A. Rubio, J.A. Alonso y P.M. Ajayan
Advanced Materials **11**, 154-157 (1999) 213 citas
- 10 P.M. Echenique, J.M. Pitarke, E.V. Chulkov y A. Rubio
Chemical Physics **251**, 1-35 (2000). 202 citas
11. Y. Miyamoto, A. Rubio, M.L. Cohen y S.G. Louie,
Physical Review B **50**, 4976 (1994) 174 citas
12. V.H. Crespi, M.L. Cohen y A. Rubio,
Physical Review Letters **79**, 2093-2096 (1997) 166 citas
- 13 A. Mujica, A. Rubio, A. Muoz y R. J. Needs, Reviews of Modern Physics **75** 863-912 (2003) 165 citas
14. J.M. Nugent, K.S.V. Santhanam, A. Rubio y P.M. Ajayan
Nano Letters **1**, 87-91 (2001) 138 citas
15. O. Zakharov, A. Rubio, X. Blase, M.L. Cohen y S.G. Louie
Physical Review B **50**, 10780 (1994) 123 citas
16. X. Blase, A. Rubio, S. G. Louie y M. L. Cohen,
Physical Review B **51**, 6868-6875 (1995) 122 citas
17. Y. Miyamoto, A. Rubio, X. Blase, M.L. Cohen y S.G. Louie
Physical Review Letters **74**, 2993-2996 (1995) 118 citas
18. 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, Advanced Materials **12**, 213-216 (2000) 117 citas
19. Y. Miyamoto, A. Rubio, M.L. Cohen y S.G. Louie,
Physical Review B **50** 18360 (1994) 115 citas
20. A. Rubio, D. Sánchez-Portal, E. Artacho, P. Ordejón y J.M. Soler
Physical Review Letters **82**, 3520-3523 (1999). 115 citas
21. E. Hernández, C. Goze, P. Bernier y A. Rubio,
Applied Physics A **68** 287-292 (1999) 115 citas
22. A. Rubio, J.A. Alonso, X. Blase, L.C. Balbás y S.G. Louie
Physical Review Letters **77**, 247-250 (1996) 100 citas

- In total more than 9900 cites: Index h=50;
- ISI Essential Science Indicators in Physics, Chemistry and Materials Science (<http://isiknowledge.com>).
- The work A. Rubio *et al.* Physical Review Letters **77**, 247-250 (1996) and X. Blase *et al.* Physical Review (Rapid Communications) B **52**, 2225 (1995) was highlighted as “Perspectives in Science: Condensed Matter Physics”, Science **273**, 751 (1996).
- The works A. Rubio *et al.* Physical Review B **49**, 5081-5084 (1994); **53**, 4023-4026 (1996) were highlighted in Science **280**, 545 (1998) (Applied Physics: “Nanowires: Small is Beautiful”).
- Creation of the octopus project in collaboration with M.A.L. Marques, A Castro and G.F. Bertsch. The computer project is aimed at describing the excited state electron-ion dynamics in finite (nanostructures) and extended systems under the influence of time-dependent electromagnetic fields or arbitrary intensity, duration and shape. The program can be freely downloaded from <http://www.tddft.org/programs/octopus>
- The work published in Nature Materials (C. Gómez-Navarro *et al.*, **4** 534-539 (2005)) got a News and Views, Nature Materials (Vol.4, pag. 514-515) and selected as “hot paper in materials science” (November 2006),
- The work *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); was selected as one of the most important articles in physics in the last years (ISI Essential Science Indicators <http://go5.isiknowledge.com/portal.cgi>). Moreover in September 2008 was identified by Thomson Reuters’ Essential Science Indicators to be one of the most cited papers in the field of Physics (see <http://ScienceWatch.com>)
- Many works have been selected and cited by nanotechweb.org (from the Institute of Physics Publishing that serves the global nanotechnology community) and “Virtual Journal of Nanoscale Science and Technology” (<http://www.vjnano.org>)

Collaborators and other affiliations

- Collaborators in USA: S.G. Louie, M.L. Cohen, G.F. Bertsch, P.M. Ajayan, D.L. Carroll, T. Hertel, H. Petek, V.H. Crespi, D. Luzzi, D. Tomanek.
- Collaborators in Japan: S. Iijima, K. Yabana, Y. Miyamoto, S. Saito, K. Ishioka.
- Collaborators in Europe (not in San Sebastián): L. Reining, G. Onida, R.W. Godby, R. del Sole, E.K.U. Gross, P. Bernier, S. Roth, A. Loiseau, R. Nieminen, M. Wolf, T. Pichler.
- **Postdoctoral** Fellows Sponsored by European Community now with permanent positions: S. Roche (U. Grenoble), F. Rabilloud (U. Lyon), C. Goze (U. Montpellier), E. Hernández (U. Barcelona), M.A.L. Marques (Coimbra), L. Wirtz (Lille, France), F. Sottile (Paris), A. Mrini (Rome). Present K. Thygesen, M. Gruning, Y. Pouillon.
On Sabbatical: I. Boustani (U. Wuppertal), N.H. March (U. Oxford), M.J. Stott (Queen’s U.) **PhD Students:** X. Andrade, M. Oliveira, A. Castro (FU-Berlin), D. Varsano (S3, Modena), R. Arenal de la Concha (U. Paris), J. Serrano (Grenoble), T. del Caño, S. Latyl (now in U. Namur).

Selected Recent List of Publications

1. L. Wirtz, A. Marini, and A. Rubio *Excitons in boron nitride nanotubes: dimensionality effects* Physical Review Letters **96** 126104-1,4 (2006)
2. J.F. Dobson, A. White and A. Rubio *Asymptotics of the dispersion interaction: analytic benchmarks for van der Waals energy functionals* Physical Review Letters **96** 073201-1,4 (2006)
3. B. Biel, F.J. Garcia-Vidal, A. Rubio and F. Flores *Anderson localization in carbon nanotubes: defect density and temperature effects* Physical Review Letters **95**, 266801-1,4 (2005)
4. 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 (19th-June-2005)
5. 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)

6. X. López, M.A.L. Marques, A. Castro and A. Rubio, *Optical Absorption in the Blue Fluorescent Protein: a First Principles Study*, Journal of the American Chemical Society **127**, 12329-12337 (2005)
7. Y. Miyamoto, N. Jinbo, H. Nakamura, A. Rubio, and D. Tománek *Photodesorption of Oxygen from Nanotubes* Physical Review B (Brief Report) **70** 233408-1,4 (2004)
8. F. Triozon, S. Roche, A. Rubio and D. Mayou *Electrical transport in carbon nanotubes: role of disorder and helical symmetries* Physical Review B (Rapid Communications) **69** R121410-1,4 (2004)
9. A. Marini, R. Del Sole and A. Rubio *Bound excitons in time-dependent density-functional-theory: optical and energy-loss spectra* Physical Review Letters **91**, 256402-1,4 (2003)
10. M.A.L Marques, X. Lopez, D. Varsano, A. Castro, and A. Rubio *Time-Dependent Density-functional approach for biological photoreceptors: the case of the Green Fluorescent Protein* Physical Review Letters **90**, 158101-1,4 (2003)
11. 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)
12. A.G. Marinopoulos, L. Reining, A. Rubio, and N. Vast *Optical and loss spectra of carbon nanotubes: Depolarization effects and intertube interactions* Physical Review Letters **91**, 046402-1,4 (2003)
13. G. Onida, L. Reining and A. Rubio, *Electronic Excitations: Density-Functional versus Many-body Green's-Functions Approaches* Reviews of Modern Physics **74** 601-659 (2002)
14. L. Reining, V. Olevano, A. Rubio and G. Onida *Excitonic effects in solids described by time-dependent density functional theory* Physical Review Letters **88** 066404-1,4 (2002)