

Name: **Riccardo RURALI**
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Qualifications

- Degree in Electrical Engineering (Optoelectronics) achieved at the Politecnico di Milano the 15/10/96. Graduation mark 96/100.
- Habilitation to work as an engineer according to Italian law (Esame di Stato, May 1996).
- PhD in Materials Science *cum laude* at the Universitat Autònoma de Barcelona. 17/12/2003.

Professional and academic experience

- **Politecnico di Milano**
Milan, Italy (1990 – 1997)

Degree in Electrical Engineering (Optoelectronics) at the Politecnico di Milano. Graduation mark of 96/100.

Graduation Thesis at the Dipartimento di Fisica of the Politecnico di Milano (supervisor Prof. G. Consolati ; September 1995 - October 1996): *Free volume determination in polymeric materials through positron annihilation spectroscopy*.

Stay at the Positron Annihilation group of the Subatomic and Radiation Department at Rijksuniversiteit Gent, Belgium (supervisor Prof. C.A. Dauwe) to carry out part of the work of the Graduation Thesis (April 1996 – June 1996).

Postgraduate training at the Dipartimento di Fisica of the Politecnico di Milano, as a collaborator of the Positron Annihilation group (October 1996 – April 1997).

- **ABB - Asea Brown Boveri**
Milan, Italy and Västerås, Sweden (1998 - 2000)

Master in Business Administration (MBA) at SDA Bocconi Business school (Milan), sponsored by ABB Italia (January 1998 - April 1998).

ABB Industria, Automation and Drives division, Milan (Italy). Process automation (May 1998 - December 1998 and February 2000 – July 2000).

ABB Industrial Systems, Automation and Drives division, Västerås (Sweden). Mathematical modeling and simulation of coil eccentricity compensation (January 1999 – January 2000).

- **Consejo Superior de Investigaciones Científicas – CSIC**
Barcelona, Spain (2000 – 2003)

PhD in Materials Science *cum laude* at the Universitat Autònoma de Barcelona.

Doctoral Thesis at the Centro Nacional de Microelectrónica and at the Institut de Ciència dels Materials de Barcelona, institutes of the Spanish National Council of Research (supervisors Dr. E. Hernández and Prof. P. Godignon; September 2000 – December 2003): *Theoretical modelling of defects in silicon carbide*.

- **Université Paul Sabatier**
Toulouse, France (2004 – 2005)

Postdoc at the Laboratoire Collisions, Agrégats, Réactivité in the group of Prof. N. Lorente.
Electronic structure of nanowires, inelastic scattering of molecules on surfaces, simulations of STM images.

- **Universitat Autònoma de Barcelona**
Barcelona, Spain (2006 – 2009)

Postdoc at the Escola Tècnica Superior d'Enginyeria (ETSE) in the group of Prof. J. Suñé.
Electron transport in nanowires, nanoelectronics devices and sensors based on nanowires, materials for spintronics.

- **Consejo Superior de Investigaciones Científicas – CSIC**
Barcelona, Spain (2009 – today)

Tenured Scientist at the Institut de Ciència de Materials de Barcelona (ICMAB-CSIC).

Grants and fellowships

- Three-month ERASMUS scholarship of the European Union (EU) for a stay at the University of Ghent (Belgium). April 1996 – June 1996.
- Pre-doctoral grant through ATOMCAD, a Research and Training Network (RTN) of the European Union (EU), to carry out the PhD studies at the Universitat Autònoma de Barcelona (Spain). September 2000 – December 2003
- Two-year postdoctoral grant of the Generalitat de Catalunya (NANOTEC) to work at the Université Paul Sabatier, Toulouse (France). January 2004 – December 2005.
- Juan de la Cierva contract of the Ministerio de Educación y Ciencia to work at the Universitat Autònoma de Barcelona (Spain). January 2006 – December 2007.
- Ramón y Cajal contract of the Ministerio de Educación y Ciencia to work at the Universitat Autònoma de Barcelona (Spain). January 2008 – today.

Computer skills and code development

Programming languages: C, Fortran90 and Pascal. Operative systems: Linux, MS-DOS and Windows at user level.

Experience in empirical potential, tight-binding and density-functional theory calculations (TROCADERO, SIESTA, DACAPO, VASP).

Development for large-scale computer code projects [R. Rurali and E. Hernández, *Comp. Mat. Sci.*, **28**, 85-106 (2003)]: Tersoff inter-atomic empirical potential for silicon, carbon and silicon carbide, environment dependent empirical potential (EDIP) for silicon, calculation of the vibrational density of states.

Languages

- Italian native language
- Excellent knowledge of written and spoken English (TOEFL certificate)
- Excellent knowledge of written and spoken Spanish
- Excellent knowledge of written and spoken Catalan (*Nivell C* qualification)
- Good knowledge of French
- Basic knowledge of Swedish

Publications

G. Consolati, R. Rurali, and M. Stefanetti, *An experimental test on the distribution of positronium lifetimes in polymers*, *Chemical Physics*, **237**, 493-499 (1998).

R. Rurali, E. Hernández, P. Godignon, J. Rebollo, and P. Ordejón, *Ab initio calculations of B diffusion in SiC*, *Materials Science Forum*, **389-393**, 553-556 (2002).

R. Rurali, P. Godignon, J. Rebollo, P. Ordejón, and E. Hernández, *Theoretical evidence for the kick-out mechanism for B diffusion in SiC*, *Applied Physics Letters*, **81**, 2989-2991 (2002).

J. L. Mozos, R. Rurali, G. Canto, E. Canadell, P. Ordejón, and E. Hernández, *Recent applications of simulation techniques in materials science and nanotechnology in Recent Research Development in Applied Physics*, Transworld Research Network (Kerala, 2003).

R. Rurali, E. Hernández, P. Godignon, J. Rebollo, and P. Ordejón, *First principles studies of neutral vacancies diffusion in SiC*, *Computational Materials Science*, **27**, 36-42 (2003).

R. Rurali, P. Godignon, J. Rebollo, E. Hernández, and P. Ordejón, *First-principles study of n-type dopants and their clustering in SiC*, *Applied Physics Letters*, **82**, 4298-4300 (2003).

R. Rurali, E. Hernández, P. Godignon, J. Rebollo, and P. Ordejón, *First principles studies of n and p dopant interactions in SiC: implications for co-doping*, *Materials Science Forum*, **433-436**, 649-652, (2003).

E. Hernández, V. Meunier, B. W. Smith, R. Rurali, H. Terrones, M. Buongiorno Nardelli, M. Terrones, D. E. Luzzi, and J. -C. Charlier, *Fullerene coalescence in nanopeapods: a path to novel tubular carbon*, *Nano Letters* **3**, 1037-1042 (2003).

R. Rurali and E. Hernández, *Trocadero: a multi-algorithm multi-model approach*, *Computational Materials Science*, **28**, 85-106 (2003).

U. Gerstmann, P. Deák, R. Rurali, B. Aradi, Th. Frauenheim, and H. Overhof, *Charge correction to supercell calculations of defects in semiconductors*, *Physica B*, **340**, 190-194 (2003).

- R. Rurali, E. Wachovicz, P. Ordejón, P. Godignon, J. Rebollo, and P. Hyldegaard, *First-principles adsorption of O at SiC surface*, Materials Science Forum, **457-460**, 1293-1296, (2003).
- R. Rurali, P. Godignon, J. Rebollo, P. Ordejón, and E. Hernández, *Self-passivation mechanisms in clusters of n dopants in SiC*, physica status solidi (c), **1**, 274-277 (2004).
- G. Karwasz, R. Rurali, G. Consolati, and P. Godignon, *Defect dynamics in P-implanted 6H-SiC studied by positron annihilation spectroscopy*, physica status solidi (c), **1**, 257-260 (2004).
- R. Rurali, E. Hernández, P. Godignon, J. Rebollo, and P. Ordejón, *First-principles studies of the diffusion of B impurities and vacancies in SiC*, Physical Review B **69**, 125203 (2004).
- M. Kaczmarek, R. Rurali, and E. Hernández, *Reversible scaling simulation of the melting transition in silicon*, Physical Review B **69**, 214105 (2004).
- M. Kaczmarek, R. Rurali, and E. Hernández, *Reversible scaling free energy calculations in silicon*, Proc. of the 3rd International Conference on Computational Modelling and Simulation of Materials.
- R. Rurali and N. Lorente, *Metallic and semimetallic <100> silicon nanowires*, Physical Review Letters **94**, 026805 (2005).
- K. S. Troche, V. R. Coluci, S. F. Braga, D. D. Chinellato, F. Sato, S. B. Legoas, R. Rurali, and D. S. Galvão, *Prediction of ordered phases of encapsulated C₆₀, C₇₀, and C₇₈ inside carbon nanotubes*, Nano Letters **5**, 349 (2005).
- E. Wachovicz, R. Rurali, P. Ordejón, and P. Hyldegaard, *First stages of the oxidation of the Si-rich 3C-SiC(001) surface*, Computational Materials Science **33**, 13-19 (2005).
- N. Lorente, R. Rurali, and H. Tang, *Single-molecule manipulation and chemistry with the STM*, Journal of Physics: Condensed Matter **17**, S1049-S1074 (2005).
- R. Rurali and N. Lorente, *On the properties of surface reconstructed silicon nanowires*, Nanotechnology **16**, S250-S253 (2005).
- R. Rurali, *Electronic and structural properties of silicon carbide nanowires*, Physical Review B **71**, 205405 (2005).
- R. Rurali, N. Lorente, and P. Ordejón, *Comment on "Molecular distortions and chemical bonding of a large π -conjugated molecule on a metal surface"*, Physical Review Letters **95**, 209601 (2005).
- J. Kröger, N. Néel, H. Jensen, R. Berndt, R. Rurali, and N. Lorente, *Molecules on vicinal Au surfaces studied by STM*, Journal of Physics: Condensed Matter **18**, S51-S66 (2006).
- R. Rurali, V. R. Coluci, and D. S. Galvão, *Prediction of giant electroactuation for papyruslike carbon nanoscroll structures: First-principles calculations*, Physical Review B **74**, 085414 (2006).
- I. Fernández-Torrente, K. J. Franke, N. Henningsen, G. Schulze, M. Alemani, Ch. Roth, R. Rurali, N. Lorente, and J. I. Pascual, *Spontaneous formation of triptycene supramolecules on surfaces*, Journal of Physical Chemistry B **110**, 20089-20092 (2006).
- R. Rurali, A. Poissier, and N. Lorente, *Size effect in surface-reconstructed <100> and <110> silicon nanowires*, Physical Review B **74**, 165324 (2006).
- M. Berthe, A. Urbieto, L. Perdigão, B. Grandidier, D. Deresmes, C. Delerue, D. Stiévenard, R. Rurali, N. Lorente, L. Magaud, and P. Ordejón, *Polaron transport through interface atoms*, Physical Review Letters **97**, 206801 (2006).
- T. Markussen, R. Rurali, M. Brandbyge, and A.-P. Jauho, *Mean free path in silicon nanowires: Role of surface disorder*, Physical Review B **74**, 245313 (2006).
- R. Rurali, J. Suñé, and X. Cartoixà, *Ordered arrays of quantum wires through hole patterning: ab initio and empirical electronic structure calculations*, Applied Physics Letters **90**, 083118 (2007).
- J. Kröger, H. Jensen, R. Berndt, R. Rurali, and N. Lorente, *Molecular orbital shift of perylenetetracarboxylic-dianhydride*, Chemical Physics Letters **438**, 249-253 (2007); cond-mat/0506025.
- K. S. Troche, V. R. Coluci, R. Rurali, and D. S. Galvão, *Structural and electronic properties of zigzag carbon nanotubes filled with small fullerenes*, Journal of Physics: Condensed Matter **19**, 236222-236231 (2007).

- T. Markussen, R. Rurali, A.-P. Jauho, and M. Brandbyge, *Scaling theory put into practice: First-principles modeling of transport in doped silicon nanowires*, Physical Review Letters **99**, 076803 (2007).
- R. Rurali, B. Aradi, Th. Frauenheim, and A. Gali, *Accurate single-particle determination of the band gap in silicon nanowires*, Physical Review B **76**, 113303 (2007).
- J. M. Pruneda, V. Ferrari, R. Rurali, P. B. Littlewood, N. A. Spaldin, and E. Artacho, *Ferrodistorive instability at the (001) surface of half-metallic manganites*, Physical Review Letters **99**, 226101 (2007).
- R. Rurali, X. Cartoixà, and D.S. Galvão, *Large electromechanical response in silicon nanowires predicted from first-principles electronic structure calculations*, Physical Review B **77**, 073403 (2008).
- X. Cartoixà, R. Rurali, I. Fernández-Cuesta, F. Pérez-Murano, and J. Suñé, *Fabrication of ordered arrays of quantum wires through hole patterning*, Journal of Physics: Conference Series **100**, 052049 (2008).
- A. Barreiro, R. Rurali, E. R. Hernández, J. Moser, T. Pichler, L. Forró, and A. Bachtold, *Subnanometer motion of cargoes driven by thermal gradients along carbon nanotubes*, Science **320**, 775-778 (2008).
- T. Markussen, R. Rurali, A.-P. Jauho, and M. Brandbyge, *Transport in silicon nanowires: role of radial dopant profile*, Journal of Computational Electronics **7**, 324-327 (2008).
- R. Rurali, T. Markussen, J. Suñé, M. Brandbyge, and A.-P. Jauho, *Modeling transport in ultrathin Si nanowires: Charged versus neutral impurities*, Nano Letters **8**, 2825-2828 (2008).
- N. Henningsen, R. Rurali, K. J. Franke, I. F. Torrente, and J. I. Pascual, *Trans to cis isomerization of azobenzene on Cu(100)*, Applied Physics A **93**, 241-246 (2008).
- X. Cartoixà and R. Rurali, *The BN-pair impurity in carbon nanotubes and the possibility for disorder-induced frustration of gap formation*, Nanotechnology **19**, 445709 (2008).
- G. Giorgi, X. Cartoixà, A. Sgamellotti, and R. Rurali, *Mn-doped silicon nanowires: First-principles calculations*, Physical Review B **78**, 115327 (2008).
- R. Rurali, E. Wachowicz, P. Hyldgaard, and P. Ordejón, *Band bending and quasi-2DEG in the metallized β -SiC(001) surface*, physica status solidi - Rapid Research Letters **2**, 218-220 (2008).
- R. Rurali and X. Cartoixà, *Theory of Defects in One-Dimensional Systems: Application to Al-Catalyzed Si Nanowires*, Nano Letters **9**, 975-979 (2009).
- R. Rurali, B. Aradi, Th. Frauenheim, and A. Gali, *Donor levels in Si nanowires determined by hybrid-functional calculations*, Physical Review B **79**, 115303 (2009).
- R. Rurali, R. Cuadrado, and J. I. Cerdá, *C_{60} adsorption on the Si(111)-p(7 \times 7) surface: A theoretical study*, Physical Review B **81**, 075419 (2010).
- X. Cartoixà, R. Rurali, I. Fernández-Cuesta, F. Pérez-Murano, and J. Suñé, *Fabrication of ordered arrays of quantum wires through hole patterning*, Journal of Physics Conference Series **100**, 052049 (2008).
- Y. Gebremichael, A. Sánchez, X. Borrisé, M. Schmidt, A. R. Goñi, M. I. Alonso, R. Rurali, J. Suñé, X. Cartoixà, and F. Pérez-Murano, *Pattern transfer optimization for the fabrication of arrays of silicon nanowires*, Microelectronic Engineering **87**, 1479-1482 (2010).
- T. Markussen, R. Rurali, X. Cartoixà, A.-P. Jauho, and M. Brandbyge, *Scattering cross section of metal catalyst atoms in silicon nanowires*, Physical Review B **81**, 125307 (2010).
- R. Rurali, Colloquium: *Structural, electronic, and transport properties of silicon nanowires*, Reviews of Modern Physics **82**, 427-449 (2010).
- R. Rurali, M. Palumbo, and X. Cartoixà, *Convergence study of neutral and charged defect formation energies in Si nanowires*, Physical Review B **81**, 235304 (2010).
- R. Rurali and E. R. Hernández, *Thermally induced directed motion of fullerene clusters encapsulated in carbon nanotubes*, Chemical Physics Letters **497**, 62-65 (2010).
- Á. Miranda-Durán, X. Cartoixà, M. Cruz Irisson, and R. Rurali, *Molecular Doping and Subsurface Dopant Reactivation in Si Nanowires*, Nano Letters **10**, 3590-3595 (2010).

- F. D. Novaes, R. Rurali, and P. Ordejón, *Electronic Transport between Graphene Layers Covalently Connected by Carbon Nanotubes*, ACS Nano **4**, 7596-7602 (2010).
- N. Henningsen, R. Rurali, C. Limbach, R. Drost, J. I. Pascual, and K. J. Franke, *Site-Dependent Coordination Bonding in Self-Assembled Metal–Organic Networks*, Journal of Physical Chemistry Letters **2**, 55-61 (2011).
- M. Amato, S. Ossicini, and R. Rurali, *Band-Offset Driven Efficiency of the Doping of SiGe Core-Shell Nanowires*, Nano Letters **11**, 594–598 (2011).
- A. Barreiro, R. Rurali, E. R. Hernández, and A. Bachtold, *Structured Graphene Devices for Mass Transport*, Small **7**, 775-780 (2011).
- M. López-Suárez, R. Rurali, L. Gammaitoni, and G. Abadal, *Nanostructured graphene for energy harvesting*, Physical Review B **84**, 161401(R) (2011).
- J. Chaste, A. Eichler, J. Moser, G. Ceballos, R. Rurali, and A. Bachtold, *A nanomechanical mass sensor with yoctogram resolution*, Nature Nanotechnology **7**, 301–304 (2012).
- M. de la Mata, C. Magen, J. Gazquez, M. I. B. Utama, M. Heiss, S. Lopatin, F. Furtmayr, C. J. Fernández-Rojas, B. Peng, J. R. Morante, R. Rurali, M. Eickhoff, A. Fontcuberta i Morral, Q. Xiong, and J. Arbiol, *Polarity Assignment in ZnTe, GaAs, ZnO, and GaN-AlN Nanowires from Direct Dumbbell Analysis*, Nano Letters **12** (5), 2579–2586 (2012).
- Á. Miranda, A. Trejo, E. Canadell, R. Rurali, M. Cruz-Irisson, *Interconnection effects on the electronic and optical properties of Ge nanostructures: A semi-empirical approach*, Physica E **44** (7-8) 1230–1235 (2012).
- M. Amato, S. Ossicini, and R. Rurali, *Electron Transport in SiGe Alloy Nanowires in the Ballistic Regime from First-Principles*, Nano Letters **12** (6), 2717–2721 (2012).
- Á. Miranda, X. Cartoixà, E. Canadell, and R. Rurali, *NH₃ Molecular Doping of Silicon Nanowires grown along the [112], [110], [001] and [111] orientations*, Nanoscale Research Letters **7**, 308 (2012).
- B. Yan, R. Rurali, and Á. Gali, *Ab Initio Study of Phosphorus Donors Acting as Quantum Bits in Silicon Nanowires*, Nano Letters **12** (7), 3460–3465 (2012).
- M. Amato, R. Rurali, and S. Ossicini, *Doping of SiGe core-shell nanowires*, Journal of Computational Electronics **11** (3), 272-279 (2012).
- X. Cartoixà, R. Rurali, and J. Suñé, *Transport properties of oxygen vacancy filaments in metal/crystalline or amorphous HfO₂/metal structures*, Physical Review B **86**, 165445 (2012).
- M. Amato, M. Palumbo, R. Rurali, and S. Ossicini, *Optical absorption modulation by selective codoping of SiGe core-shell nanowires*, Journal of Applied Physics **112**, 114323 (2012).
- M. López-Suárez, R. Rurali, and G. Abadal, *Buckling suspended graphene nanoribbons to harvest energy from noisy vibrations*, Microelectronic Engineering **111**, 122-125 (2013).
- M. López-Suárez, J. Agustí, F. Torres, R. Rurali, G. Abadal, *Inducing bistability with local electret technology in a microcantilever based non-linear vibration energy harvester*, Applied Physics Letters **102**, 153901 (2013).
- S. Long, X. Lian, C. Cagli, X. Cartoixà, R. Rurali, E. Miranda, D. Jiménez, L. Perniola, M. Liu, and J. Suñé, *Quantum-size effects in hafnium-oxide resistive switching*, Applied Physics Letters **102**, 183505 (2013).
- T. R. Umbach, I. Fernández-Torrente, M. Ruby, F. Schulz, C. Lotze, R. Rurali, M. Persson, J. I. Pascual, and K. J. Franke, *Atypical charge redistribution over a charge-transfer monolayer on a metal*, New Journal of Physics **15**, 083048 (2013).
- N. Fukata, J. Kaminaga, R. Takiguchi, R. Rurali, M. Dutta, and K. Murakami, *Interaction of Boron and Phosphorus Impurities in Silicon Nanowires during Low-Temperature Ozone Oxidation*, Journal of Physical Chemistry C **117** (39), 20300–20307 (2013).

G. Amato, A. Cultrera, L. Boarino, C. Lamberti, S. Bordiga, F. Mercuri, X. Cartoixà, and R. Rurali, *Molecular doping and gas sensing in Si nanowires: From charge injection to reduced dielectric mismatch*, Journal of Applied Physics **114**, 204302 (2013).

M. Mongillo, P. Spathis, G. Katsaros, S. De Franceschi, P. Gentile, R. Rurali, and X. Cartoixà, *PtSi clustering in silicon probed by transport spectroscopy*, Physical Review X **3**, 041025 (2013).

M. Amato, M. Palummo, R. Rurali, and S. Ossicini, *Silicon–Germanium Nanowires: Chemistry and Physics in Play, from Basic Principles to Advanced Applications*, Chemical Reviews **114**, 1371-1412 (2014).

L. Cabana, B. Ballesteros, E. Batista, C. Magén, R. Arenal, J. Oro-Solé, R. Rurali, and G. Tobias, *Template assisted growth of single-layered inorganic nanotubes*, Advanced Materials, accepted.

A. R. Goñi, L. R. Muniz, J. S. Reparaz, M. I. Alonso, M. Garriga, A. F. Lopeandia, J. Rodríguez-Viejo, J. Arbiol, and R. Rurali, *Using high pressure to unravel the mechanism of visible emission in amorphous Si/SiO_x nanoparticles*, Physical Review B **89**, 045428 (2014). Highlighted as **Editors' Suggestion**.

Popular science articles

R. Rurali, *Silicon nanowires: better if longer*. UAB Divulg@, electronic journal of popular science.

R. Rurali, *Nanoelectronics*, Investigación y Ciencia, Spanish edition of Scientific American. February 2008. Invited introductory article on silicon nanowires.

R. Rurali, E. R. Hernández, A. Barreiro, and A. Bachtold, *Consiguen desplazar objetos nanométricos mediante cambios de temperatura*. UAB Divulg@, electronic journal of popular science.

E. R. Hernández, R. Rurali, A. Barreiro, and A. Bachtold, *Nanomotores térmicos*. Investigación y Ciencia, Spanish edition of Scientific American. February 2008. Invited article.

R. Rurali, *Nanoscale energy harvesting with graphene*. NANOENERGY Letters **3**, 6 (2012), <http://www.nanopwr.eu/node/88>.

Attendance to courses and conferences

28th Polish Seminar on Positron Annihilation. 8-13 September 1996, Jarnołtówek (Poland). Attendance.

Summer School of Computational Materials Science, organized by the Advanced Studies Institute of NATO. 9-22 June 2001, Lucca (Italy). Attendance.

International Workshop on Total Energy Methods in Computational Condensed Matter. 10-12 January 2002, La Laguna (Spain). Attendance.

SIESTA meeting. September 2001, Madrid (Spain). Oral contribution.

International Conference on Silicon Carbide and Related Materials (ICSCRM 2001). 28 October - 2 November 2001, Tsukuba (Japan). Poster.

Spring Meeting of the European Materials Society (E-MRS Spring Meeting). 18-22 June 2002, Strasbourg (France). Poster.

European Conference on Silicon Carbide and Related Materials (ECSCRM 2002). 1-5 September 2002, Linköping (Sweden). Poster.

Course of Molecular dynamics of proteins and nucleic acids. Les Heures, Fundació Bosch i Gimpera and Universitat de Barcelona. 31 March - 4 April 2003, Barcelona (Spain). Attendance.

Fall Meeting of the European Materials Society (E-MRS Fall Meeting). 15-19 September 2003, Warsaw (Poland). Poster.

Jornades Franco-Catalanes de Nanociència i Nanotecnologia, 5-6 July 2004, Barcelona (Spain). Attendance.

Trends in Nanotechnology (TNT2004). 13-17 September 2004, Segovia (Spain). Oral contribution.

2nd NanoSpain workshop. 14-17 March 2005, Barcelona (Spain). Oral contribution.

Trends in Nanotechnology (TNT2005). 29 August-2 September 2005, Oviedo (Spain). Poster.

3rd NanoSpain workshop. 20-23 March 2006, Pamplona (Spain). Poster.

Spin and Charge Effects at the Nanoscale (SCEN06). 1-9 June 2006, Pisa (Italy). Poster.

Perspective in Nanotechnology (Nano2006), 2-4 September, Donostia (Spain). Oral contribution.

13th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods. 11-13 January 2007, Trieste (Italy). Poster.

Condensed Matter and Materials Physics (CMMP2007), 12-13 April 2007, Leicester (UK). Oral contribution.

Materials Research Society (MRS) Fall Meeting, 1-5 December 2008, Boston, MA (USA). Oral contribution.

Nanomediterraneo. 19 June 2009, Castelló de la Plana (Spain). Attendance.

IEEE NANO 09. 26-30 Julio 2009, Genoa (Italy). Invited oral contribution.

Trends in Nanotechnology (TNT2009). 7-11 September 2009, Barcelona (Spain). Oral contribution.

Optimization in Stochastic Nano-Systems. 10-13 October 2010, Hanse-Wissenschaftskolleg, Delmenhorst (Germany). Invited oral contribution.

14th International Workshop on Computational Electronics (IWCE2010). 27-29 October 2010, Consiglio Nazionale delle Ricerche (CNR), Pisa (Italy). Invited oral contribution.

CECAM / ZCAM workshop on Charge and spin transport in chemically modified graphene-based materials. 7-8 April 2011, Hotel Campus, Bellaterra (Spain). Oral contribution.

CECAM workshop on Thermal and electronic transport at the nanoscale. 20-22 June 2011, Università della Svizzera Italiana, Lugano (Switzerland). Invited oral contribution.

Third NaNoNetworking Summit – N³ Summit 2011. 22-23 June 2011, Universitat Politècnica de Catalunya, Barcelona (Spain). Invited oral contribution.

BNC-b Research Meeting. 14 July 2011, Hotel Campus, Bellaterra (Spain). Oral presentation.

Nano and Giga Challenges in Electronics, Photonics and Renewable Energy (NG2011). 12-16 September 2011, Lomonosov Moscow State University, Moscow (Russia). Oral presentation.

GdR Nanofils Semiconducteurs. 17-21 October 2011, Village Club IGESA, Porquerolles (France). Invited oral presentation.

Electronic Material Conference (EMC) MRS Workshop Series. 20-22 June 2012, Pennsylvania State University, State College, PA (USA). Oral presentation.

NANOSELECT Meeting. 1-4 July 2012, Hotel Eden Roc, Sant Feliu de Guixols (Spain). Invited oral presentation.

International Conference on Nanoscience + Technology (ICN+T). 23-27 July 2012, La Sorbonne, Paris (France). Oral presentation.

IEEE Nano 2012. 20-23 August 2012, International Convention Centre, Birmingham (UK). Invited oral presentation.

CECAM workshop on Defects and Surfaces in Electronic Materials. 14 September 2012, BCCMS University Campus, Bremen (Germany). Invited oral presentation.

Zeropower workshop. 16-18 September 2012, Hotel Campus, Bellaterra (Spain). Oral presentation.

Materials Research Society (MRS) Fall Meeting. 25-30 November 2012, Boston, MA (USA). Invited oral presentation.

Materials Research Society (MRS) Spring Meeting. 1-5 April 2013, San Francisco, CA (USA). Oral presentation.

Italian National Conference on Condensed Matter Physics (FISMAT2013). 9-13 September 2013, Milan (Italia). Oral presentation.

International Conference on One-Dimensional Nanosystems (ICON). 23-26 September 2013, Annecy (France). Oral presentation.

Participation in projects

Pre-doctoral fellow within ATOMCAD, a Research and Training Network (RTN) of the European Union (HPRN CT 1999 00048).

Participation in the project of the Ministerio de Ciencia y Tecnología *Application of methods ab-initio order-N: realistic quantum-mechanics simulations of complex systems in materials physics, solid state chemistry and biomolecules* (BFM2000-1312-C02). Project leader Prof. P. Ordejón (ICMAB-CSIC).

Participation in the project of the Ministerio de Ciencia y Tecnología *Application of new techniques of simulation to the study of structural, electronic and transport properties in materials physics and nanotechnology* (BFM2002-03278). Project leader Dr. E. Hernández (ICMAB-CSIC).

Participation in the project of the Ministerio de Educación y Ciencia *Nanoelectronic devices sub-45 nm: from atomistic simulation to compact modelling* (TEC2006-13731-C02-01/MIC). Project leader Prof. J. Suñé (UAB).

Participation in the project of the CSIC (Proyecto Intramural de Frontera) *Electromechanical systems based in silicon nanowires* (NanoSi – PIF06-037). Project leader Dr. A. San Paulo (CNM-CSIC).

Participation in the project *Fabrication of arrays of quantum wires through hole patterning* for accessing the Integrated Nano-Microelectronics Clean Room (ICTS) of the CNM-CSIC within the GICSERV program. Project leader Dr. X. Cartoixà (UAB).

Participation in the project “Explora” of the Ministerio de Ciencia e Innovación *Artificial Solids through hole structures*, (TEC2008-01865-E). Project leader Dr. X. Cartoixà (UAB).

Participation in the Project *Development and application of quantum-mechanical simulation methods in complex materials, nanostructures and surfaces* of the Ministerio de Ciencia e Innovación (FIS2009-12721-C04). Project leader Prof. A. García (ICMAB-CSIC).

Participation in the Project *Simulation of electron transport and its quantum correlations on nanoscale devices* of the Ministerio de Ciencia e Innovación (TEC2009-06986). Project leader Prof. X. Oriols (UAB).

Participation in the Project *First-principles atomistic simulations: methodology and applications to complex systems* of the Ministerio de Economía y Competitividad (FIS2012-37549-C05-05). Project leader Prof. A. García (ICMAB-CSIC).

Patents and technology transfer

X. Cartoixà, R. Rurali, and J. Suñé, *Method for the control of the coupling in a nanowire array*. European Patent PCT/ES2007/00068 with priority date November 27, 2007.

Short visits

Prof. P. Hyldgaard, Chalmers University, Göteborg (Sweden). February 2002. One week.

Prof. P. Hyldgaard, Chalmers University, Göteborg (Sweden). February 2004. One week.

Prof. M. Barndbyge, Danish Technology University, Lyngby (Denmark). October 2004. One week.

Dr. J. I. Cerdá, Instituto de Ciencia de Materiales de Madrid – CSIC, Madrid (Spain). December 2004. One week.

Prof. D. S. Galvão, Universidade Estadual de Campinas (Unicamp), Campinas (Brasil). April 2005. Two weeks.

Prof. J. I. Pascual, Freie Universität, Berlin (Germany). November 2005. One week.

Prof. M. Barndbyge, Danish Technology University, Lyngby (Denmark). May 2006. One week.

Prof. M. Barndbyge, Danish Technology University, Lyngby (Denmark). February 2007. One week.

Prof. M. Barndbyge, Danish Technology University, Lyngby (Denmark). November 2008. One week.

Seminars

Centro Nacional de Microelectrónica, Consejo Superior de Investigaciones Científicas, Barcelona (Spain). June 2002.

Laboratoire Collisions, Agrégats, Réactivité, Université Paul Sabatier, Toulouse (France). March 2004. Danish Technology University, Lyngby (Denmark). October 2004.

Laboratoire des Collisions Atomiques et Moléculaires, Université Paris Sud II, Orsay (France). February 2005.

Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas (Unicamp), Campinas (Brasil). April 2005.

Institut für Experimentalphysik, Freie Universität, Berlin (Germany). November 2005.

Institut für Festkörperphysik, Technischen Universität, Berlin (Germany). November 2005.

Donostia International Physics Center, Donostia (Spain). June 2006. Invited seminar.

Danish Technology University, Lyngby (Denmark). February 2007.

Instituto de Microelectronica de Madrid (IMM-CSIC). Octubre 2010. Invited seminar.

Teaching

2006/07 – 2.5 credits

Analog Electronics	Telecommunication Engineering	problems
Applied Electronics	Physics	problems
Electronic Devices	Telecommunication Engineering	problems
Instrumentation	Telecommunication Engineering	problems

2007/08 – 6.0 credits

Electron Devices	Physics	theory
Applied Electronics	Physics	problems
Applied Electronics	Physics	laboratory
Electronic and Photonic Devices	Electronics Engineering	problems

2008/09 – 6.0 credits

Electronics	Physics	theory
Applied Electronics	Physics	problems
Applied Electronics	Physics	laboratory
Electronic and Photonic Devices	Electronics Engineering	problems
Master in Nanoelectronics Devices		

2009/2010

Master in Nanoelectronics Devices
Master in Nanotechnology

Member of the Jury of the Research Project of the Master in Nanotechnology of Alfonso Alarcón Pardo, Universitat Autònoma de Barcelona.

Member of the PhD Thesis jury of Guillermo Albareda Piquer, Universitat Autònoma de Barcelona: *Classical and Quantum Trajectory-based Approaches to Electron Transport with full Coulomb Correlations*.

Member of the PhD Thesis jury of Álvaro Miranda Durán, Instituto Politécnico Nacional: *Estudio de las propiedades electrónicas y dieléctricas de nanoestructuras tipo zinc-blenda*.

Member of the PhD Thesis jury of Marianna Sledzinska, Institut Català de Nanotecnologia (ICN): *Carbon nanotube nanoelectromechanical Systems*.

Supervision of students and scientific visit

Direction of the stage of master-I of the Licence en Physique of Adrien Poissier at the Université Paul Sabatier. *Calcul de la structure électronique de nanofils de silicium*.

Direction of the *Prácticas de Empresa* of Miquel López Suárez within the *Licenciatura de Física*, Universitat Autònoma de Barcelona. *Theoretical study of graphene – platinum junction with first-principles methods*.

Scientific supervisor of the stay of Michele Amato, PhD student at the Università di Modena e Reggio Emilia (Italy) within the HPC-Europa2 Transnational Access program. Two stays of size weeks each. *SiGe Nanowires: computational study of electronic and transport properties through ab-initio methods*

Scientific supervisor of the stay of Francesco Mercuri, staff scientist at the Università di Perugia (Italia) within the HPC-Europa2 Transnational Access program. Six weeks. *Structural, electronic and transport properties of functionalized silicon nanowires*.

Scientific supervisor of the stay of Carlos Javier Fernández, PhD student of the Universidad de los Andes (ULA), Venezuela. One year. *Electronic properties of nanoscale silicon polymorphs*.

Scientific supervisor of the stay of Eudar Batista Hernández, predoctoral student of the Centro de Estudios Avanzados de Cuba (CEAC). One year. *Structural and electronic properties of encapsulated carbon nanotubes*.

Co-direction of PhD Thesis of Miquel López Suárez, Universitat Autònoma de Barcelona. *Energy harvesting from the microscale to the nanoscale*.

Organization of workshops and conferences

Organizer of the international workshop *NW08: Structural, electronic and transport properties of quantum wires*, CECAM, Lyon (France). Approximately 50 participants from Europe, USA, Brazil and Japan. Financing 20000 € from CECAM, European Science Foundation (ESF), Ψ_k and COST networks. Co-organizers: Mads Brandbyge (DTU, Denmark) and Xavier Blase (CNRS, France).

Member of the International Steering Committee of the conference *Trends in nanomechanics and nanoengineering*, Krasnoyarsk (Russia), September 2009.

Organizer of the international workshop *NW09: Dopants and Impurities in Semiconducting Nanowires*, CECAM, Lausanne (Switzerland). Approximately 30 participants from Europe, USA, Korea and Japan. Financing 9000 € from CECAM. Co-organizers: Mads Brandbyge (DTU, Denmark) and Xavier Blase (CNRS, France).

Organizer of the international workshop *NW10*, Foundation for Research and Technology (FORTH), Heraklion (Greece). Approximately 40 participants from Europe and USA. Co-organizers: Antonis Andriotis (FORTH, Crete), Suneel Kodambaka (UCLA), and Maurizia Palummo (Università di Roma).

Organizer of the international workshop *NW11*, Cultural Center, Plomariou, Lesvos (Greece). Approximately 40 participants from Europe, Japan and USA. Co-organizers: Antonis Andriotis (FORTH, Crete) and Maurizia Palummo (Università di Roma).

Organizer of the international workshop *NW12*, Paul Drude Institute, Berlin (Germany). Approximately 90 participants from Europe, Japan, Australia and USA. Co-organizers: Lutz Geelhaar (Paul Drude Institute, Berlin), Brian A. Korgel (University of Texas at Austin) and Maurizia Palummo (Università di Roma).

Organizer of Symposium Q, *Surfaces of Nanoscale Semiconductors*, at the MRS Fall Meeting 2013. Co-organizers: Michael A. Filler (Georgia Institute of Technology), Emily A. Weiss (Northwestern University), and William A. Tisdale (Massachusetts Institute of Technology).

Organizer of the CECAM workshop *Theory, Simulation and Modelling of SiGe Nanostructures: from Nanoelectronics to Renewable Energy*, CECAM-HQ, EPFL, Lausanne (Switzerland). Co-organizers: Michele Amato (Université Paris Sud), Maurizia Palummo (Università di Roma), and Stefano Ossicini (Università di Modena e Reggio Emilia).

Organizer of the international workshop *NW13*, Weizmann Institute of Science in Rehovot (Israel). Approximately 120 participants from Europe, Japan, and USA. Co-organizers: H. Shtrikman (Weizmann Institute of Science, Rehovot), Y. Rosenwaks (Tel-Aviv University), Lutz Geelhaar (Paul Drude Institute, Berlin), Naoki Fukata (National Institute for Materials Science, Tsukuba), and Michael A. Filler (Georgia Institute of Technology).

Other merits

Young Scientist Award at the E-MRS Spring Meeting, Strasbourg (France) for the work *First principles studies of neutral vacancies diffusion in SiC*.

Referee of the following international journals: Physical Review Letters, Physical Review B, Nano Letters, ACS Nano, Journal of Physics: Condensed Matter, Nanotechnology, Europhysics Letters, Physica Status Solidi, Physica E, Journal of Nanoscience and Nanotechnology

Referee of projects for the ACS Petroleum Research Fund, the Fonds Wetenschappelijk Onderzoek — Vlaanderen (FWO) and for Tenure and Promotion of the College of Nanoscale Science and Engineering University at Albany.