MARCO BUONGIORNO NARDELLI
Curriculum Vitæ

Full Professor
Department of Physics and Department of Chemistry
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Oak Ridge National Laboratories
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Main research interests:

- computational materials and high performance simulations
- materials and processes for energy and environment applications
- nano-catalysis
- molecular electronics at the nanoscale and quantum electronic and thermal transport in molecules and complex materials
- design of novel electronic devices
- physics and materials science at interfaces and surfaces
- theoretical developments of Density Functional Theory-based methods and multiscale computational techniques

Education

1993 Ph.D. in Physics at the ``International School for Advanced Studies" (SISSA/ISAS) in Trieste, Italy, under the supervision of Prof. S. Baroni.

1991 M.Sc. in Physics at the ``International School for Advanced Studies" (SISSA/ISAS) in Trieste, Italy, under the supervision of Prof. S. Baroni.

1989 Degree (*Laurea*) in Physics *summa cum laude* at the University of Rome ``La Sapienza" under the supervision of Prof. C.M. Bertoni and Prof. G. Ciccotti.

Professional Experience

Jan. 2012 to present	Full Professor, Department of Physics and Department of Chemistry, University of North Texas, Joint Faculty Appointment, ORNL
Aug. 2009 – Jan. 2012	Full Professor, Department of Physics, North Carolina State University, Joint Faculty Appointment, ORNL
Aug. 2005 – Aug. 2009	Associate professor, Department of Physics, North Carolina State University, Joint Faculty Appointment, ORNL
Aug. 2001 – Aug. 2005	Assistant professor, Department of Physics, North Carolina State University, Joint Faculty Appointment, ORNL
Nov. 1998 – Aug. 2001	Research associate, Department of Physics, North Carolina State University; group of Prof. J. Bernholc.
Nov. 1995 – Nov. 1998	Postdoc, Department of Physics, North Carolina State University; advisor: Prof. J. Bernholc.
Nov. 1993 – Nov. 1995	Postdoc, Laboratorio INFM/TASC (Advanced Technology in Surface Science and Catalysis), Trieste, Italy, in a joint theoretical-experimental project on ``Electronic structure calculations of semiconductor micro-structures, surfaces and interfaces": advisor Prof. F. Tommasini.
Nov. 1994 – Nov. 1995	Lecturer, Department of Physics, University of Trieste, course: ``Modern methods in electronic structure theory" (graduate level).
Jan. 1995 - Jul. 1995	Postdoc, ``Laboratoire de Recherches sur les Materiaux dans leur Environnement", Université de Marne-la-Vallée, Paris, France; advisor: Prof. P. Cortona.

Honors and awards

- Fellow of the Institute of Physics, 2011.
- Fellow of the American Physical Society, 2010.
- Top Italian Scientists list (rank 43) from VIA-Academy: http://www.topitalianscientists.org/Top_italian_scientists_VIA-Academy.aspx.
- Member at large, User Executive Committee of the Center for Nanoscale Materials Sciences (CNMS), 2011-2012.
- Co-Chair, Symposium II "Theory and Computer Simulation of Materials", XIX International Materials Research Congress, Cancún, México, August 14-18, 2010
- Co-Chair, Symposium II "Theory and Computer Simulation of Materials", XVIII International Materials Research Congress, Cancún, México, August 18-22, 2009
- Chair, invited session on "Computational Science", SESAPS Meeting, Nashville, TN, November 2007

- Chair, DMP invited session on “Recent advances in the computation of optical and transport properties of nanostructures”, APS March Meeting, Baltimore, MD, March 2006
- Chair, DMP focus session on “Computational Nanoscience”, APS March Meeting, Baltimore, MD, March 2006
- Chair, DMP focus session on “Theory of dielectrics, piezoelectrics and multiferroics”, APS March Meeting, Los Angeles, CA, March 2005.
- Sigma Xi Faculty Research Award, NCSU Chapter, May 2004.
- Member, Proposal Review Committee, Center for Nanophase Materials Sciences (CNMS), Oak Ridge National Laboratory
- Chair, DCOMP/DMP focus session on “Theory of Nanotubes”, APS March Meeting, Austin, TX, March 3-7, 2003.
- Faculty Research and Professional Development Award, North Carolina State University, $4,000, 2003.
- First Annual North Carolina State University International Research Exposition Award in recognition of ``Outstanding Research in Physics'', Raleigh, April 16, 1999.

Patents and inventions

- “BN/C nanotubes for Micro-Electro-Mechanical (MEM) applications”, M. Buongiorno Nardelli, NCSU # 000-133, June 2000.
- “Coulomb Buffer as a Method for Adjusting Band Offset and Alignment at Semiconductor/Insulator and Semiconductor/Semiconductor Interfaces”, F. Walker, R. Mc Kee, M. Buongiorno Nardelli, W.J. Shelton and M.G. Stocks, ORNL #1037, January 2002.
- “Piezoelectric and pyroelectric polymers with boron nitride backbone”, S. Nakhmanson, M. Buongiorno Nardelli and J. Bernholc, NCSU #04-011, August 2003.

Public scientific software releases

- ***WanT***, http://qe-forge.org/projects/want/, an integrated approach to ab initio electronic transport from maximally-localized Wannier functions, distributed as part of Quantum ESPRESSO.
- **DOSQC_1.0**, electronic transport properties of nanostructures from Tight-Binding Hamiltonians, available upon request at http://ermes.unt.edu.
- **AFLOWLIB.org**, a distributed materials properties repository from high-throughput ab initio calculations.

Scholarships

- C.N.R. (Italian National Research Council)-N.A.T.O. Senior Scholarship, 1995.
- A.R.E.A. di Ricerca di Trieste - Bull HN Information Systems Italia Grant for ``Electronic structure calculations of semiconductor micro-structures, surfaces and interfaces'', 1993-1995.
- C.N.R. Scholarship, 1993.

- SISSA Fellowship, 1989-1993.
- C.N.R. scholarship for ``Models and simulations in super-computer applications", 1989.

Professional Affiliations

- American Physical Society
- Materials Research Society
- SigmaXi, the Scientific Research Society

Curricular material development and courses taught

- PHYS 5450- "Solid State Physics", Spring 2013
- PHYS 3210 – "Analytical Mechanics", Fall 2012.
- PY 810 "Quantum many-body theory of materials" (new course, Fall 2008)
- HON 321 "Music and the Science of Sound" (Fall 2007, 2008, 2009, 2010, 2011, co-taught with Dr. Phill Stiles)
- PY 615 "Computational Physics of Materials" (new course, Spring 2006, 2007, 2008, 2009,2010, 2011)
- PY 205-208 "Physics for Scientists and Engineers" (Spring 2002, Spring 2003, Spring 2004, Spring 2005)
- PY610 "Modeling from the nanoscale to the macroscale" (Fall 2004)

Service to the University and Professional Societies

- Member, Personnel Committee
- Chair, Reappointment, Promotion and Tenure committee
- Chair, Physics computing committee
- Member, Advisory committee
- Member, Personnel Committee
- Member, Energy Committee
- Member, Space Committee
- Member, ad hoc Junior Faculty committee
- Member, NanoScience steering committee
- Referee for: Physical Review Letters, Physical Review B, Applied Physics Letters, Journal of Applied Physics, Journal of the American Chemical Society, European Journal of Physics, IEEE Transactions in Nanotechnology, Surface Science, Journal of Chemical Physics, Nanotechnology, Journal of Physics-Condensed Matter, Physica E, Journal of Physics and Chemistry of Solids, Computational Science & Discovery.
- Proposal reviewer for: National Science Foundation, US Department of Energy, American Chemical Society, CNMS-ORNL, US Civilian Research and Development Foundation, Royal Irish Academy, Ireland Higher Education Authority, CARIPLO foundation.

Research grants

Past

- PI: UT-Battelle-ORNL – joint faculty appointment, "Research and development in high performance computing and computational nanoscale science", $53,275/year, 8/16/2001 – 30/10/2010.
- PI: American Chemical Society – Petroleum Research Fund (ACS-PRF) research grant – type G, "*Ab initio* Theory of Electronic Transport in Carbon Nanotubes and Nanotube-based Structures", $37,500.00, 9/1/2002 – 9/1/2004.
- co-PI: NSF – NIRT (Nanoscale Interdisciplinary Research Team) program: "Reduced Degree of Freedom Predictive Methods for Control and Design of Interfaces in Nanofeatured Systems: Nanocrystalline Materials, Sensors and Composites", $100,000/year , July 2003-July 2009.
- co_PI: DoE – Office of Science – NSET: "Integrated Multiscale Modeling in Molecular Computing Devices", PI's M. Buongiorno Nardelli, J. Bernholc, $230,000/year (2005-2011).
- co-PI: ORNL-SEED - "Real Space Imaging of High Frequency Transport on the Nanoscale." PI's S. Kalinin, V. Meunier, A. P. Baddorf, M. Buongiorno Nardelli and D. B. Geohegan, $100,000 for one year (2004).
- PI: National Science Foundation-STC for Environmentally Responsible Solvents and Processes - $40,000 (2006-2007).
- co_PI: US Navy-Office of Naval Research - "Microscopic, macroscopic and multi-scale modeling of capacitor dielectrics and composites", PIs: M. Buongiorno nardelli and J. Bernholc, $480,000, (2005-2011).
- co-PI: National Science Foundation - " Spin Dynamics and Device Applications in Carbon Nanotubes", PIs M. Buongiorno Nardelli and K.W. Kim, $441,151 (2006-2009).
- co-PI: NIST - Univ. of Texas - "Nanoscale Phonon Transport for Thermal Management", PI: Ki Wook Kim, 04/08-03-09.
- co-PI: DARPA-CERA - 2008-2011, $120K for phase I (18 months) and another approx. $120K for phase II (18 months).
- co-PI: NSF-CCI "Center for Molecular Spintronics", $120K for phase I (36 months).
- PI: ARO-DURIP – 2010, First principles calculations of electronic and phononic transport: a practical tool-set for efficient design of novel materials and devices for nanoelectronic applications", $67K.

Current

- Co-PI: Topological decompositions and spectral sampling algorithms for element substitution in critical technologies, ONR-MURI, (N000141310635) $8,572,268.00; 1 month summer salary
- co_PI: US Navy-Office of Naval Research - "Microscopic, macroscopic and multi-scale modeling of capacitor dielectrics and composites", PIs: M. Buongiorno Nardelli and J. Bernholc, $140,000, (2010-2013).
- PI: SRC-CEMPI - Thermal Transport In Nanoscale Materials And Interfaces, 2013, $33,000

Pending

- Collaborative Research: Size-Dependent Optical Nonlinearities in Metal Nanoparticles - Theory, Experiment and Applications, National Science Foundation, $339,282; ½ month summer salary.
- DMREF: Computationally-driven Discovery of New Fe(II) Spin Crossover Materials with Spintronic Device Functionality, NSF, $1,472,044; lead PI.
- MRI: Acquisition of a Computer Cluster for Computational Modeling at the University North Texas, NSF, $601,000.

Group components

Post-doc

Dr. Priya Gopal
Dr. Luis Agapito (research assistant professor)
Dr. Jeevaka Weerasinghe
Dr. Laalitha Lyanage
Dr. Vivek Ranjan
Dr. Thushari Jayasekera (*former*, now Ass. Prof. at Southern Illinois Univ., Carbondale)
Dr. Matias Nunez (*former*, now at CONICET, Bariloche, Argentina)
Dr. Liping Huang (*former*, now Ass. Prof. at Rensselaer Pol. Inst.)
Dr. Gunn Kim (*former*, now Res. Prof. at SungKyunKwan University, Korea)
Dr. Aaron M. George (*former,* now in the private sector)
Dr. Milen Kostov (*former*, now Ass. Prof. at Florida State University)
Dr. Qingzhong Zhao (*former*, former research staff at NREL, now in the private sector)
Dr. Serge Nakhmanson (*former*, now research staff at Argonne Natl. Lab.)

Graduate students

Rui Dong
Yifeng Chen (*former*, graduated April 2013)
Shu Xu (*former,* graduated September 2012)
Jeff Mullen (*former,* graduated December 2011)
Sujata Paul (*former*, graduated February 2010)
Liping Yu (with Prof. J. Bernholc, Dep. of Physics, NCSU))
Mandayan Krishnan (*former*, graduated May 2009)
Matias Nunez (*former,* graduated May 2009)
Erik Santiso (*former*, now post-doc at MIT)

Undergraduate students

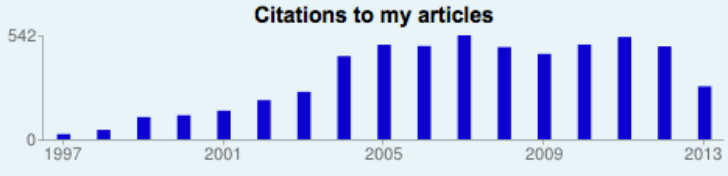
Harvey Shi (TAMS student)
(*former*) Keisha McCall (REU summer student, 2003)
(*former*) Kara Beharry (REU summer student, 2004, 2005)

PUBLICATIONS AND PRESENTATIONS

Analysis of the scientific production as of Wednesday, July 10, 2013
Source: Google Scholar
Sum of the times cited: 5655, (2714 since 2008).
h-index: 36, i-10 index: 70.
Citations per year:

Citation indices

	All	Since 2008
Citations	5655	2714
h-index	36	29
i10-index	70	55



3 most cited papers:

506 citations: K.W. Edmonds, P. Boguslawski, K.Y. Wang, R.P. Campion, S.V. Novikov, N.R.S. Farley, B.L. Gallagher, C.T. Foxon, M.Sawicki, T.Dietl, M. Buongiorno Nardelli, J. Bernholc, *Mn Interstitial Diffusion in (Ga,Mn)As*, Phys. Rev. Lett., **92**, 037201 (2004)
428 citations: M. Buongiorno Nardelli, B.I. Yakobson and J. Bernholc, *Brittle and ductile behavior in carbon nanotubes*, Phys. Rev. Lett. **81**, 4656 (1998).
434 citations: M. Buongiorno Nardelli, B.I. Yakobson and J. Bernholc, *Mechanism of strain release in carbon nanotubes*, Phys. Rev. B Rapid Communications **57**, R4277 (1998).
374 citations: M. Buongiorno Nardelli, *A general approach to electronic transport in extended systems: application to carbon nanotubes*, Phys. Rev. B, **60**, 7828 (1999).

Invited papers, review articles and books

1. S. Curtarolo, G. L. W. Hart, M. Buongiorno Nardelli, N. Mingo, S. Sanvito, and O. Levy, *The high-throughput highway to computational materials design* (invited review), Nature Materials, **12**, 191–201 (2013).
2. Erik E. Santiso, Liping Huang, Milen K. Kostov, Aaron M. George, Keith E. Gubbins and Marco Buongiorno Nardelli *Ab initio simulations of chemical reactions in nanostructured carbon materials*, in "Quantum Chemical Calculations of Surfaces and Interfaces of Materials" (Editors: V. A. Basiuk and P. Ugliengo) American Scientific Publishers, (2007).
3. M. Buongiorno Nardelli, V. Meunier and S. Nakhmanson, *Polarization in nanotubes*, in "Nanoengineering of structural materials", ed. By M. Schulz, A. Kelkar, and M. Sundaresan, CRC Press (Boca Raton, FL, 2005).
4. M. Buongiorno Nardelli and R. McKee, *Un futuro per il nanotransistor (A future for the nanotransistor)*, Le Scienze (Italian edition of "Scientific American"), **422**, 70 (2003).
5. J.-L. Fattebert and M. Buongiorno Nardelli, *Finite difference methods for ab initio electronic structure and quantum transport calculations of nanostructures*, in "Handbook of Numerical Analysis", Volume X, Special volume: Computational Chemistry, edited by C. Le Bris, Elsevier Science, (2003).

6. J. Bernholc, D. Brenner, M. Buongiorno Nardelli, V. Meunier and C. Roland, *Mechanical and electrical properties of nanotubes,* Annu. Rev. Mat. Res. **32**, 347 (2002).
7. J. Bernholc, M. Buongiorno Nardelli , J.-L. Fattebert, D. Orlikowski, C. Roland and Q. Zhao, *Mechanical Properties and Electronic Transport in Carbon Nanotubes* , edited by D. Tomanek and R. J. Enbody, Kluwer Academic Publishing, (2000).
8. J. Bernholc, M. Buongiorno Nardelli, D. Orlikowski, C. Roland and Q. Zhao, *Atomic transformations, strength, plasticity and electron transport in strained carbon nanotubes*, in ``Fiber Fracture,'' edited by M. Elices, Elsevier, (2000).
9. J. Bernholc, E. L. Briggs, C. Bungaro, M. Buongiorno Nardelli, J.-L. Fattebert, K. Rapcewicz, C. Roland, W. G. Schmidt and Q. Zhao, *Large-Scale Applications of Real-Space Multigrid Methods to Surfaces, Nanotubes, and QuantumTransport*, in ``Atomistic Modeling of Materials Properties and Phenomena'' edited by P. Deak, M. Pederson, and T. Frauenheim, Wiley-VCH (1999).
10. S. Baroni, C.M. Bertoni, M. Buongiorno Nardelli, E. Molinari, *Diagonalization of large matrices for large-scale electronic-structure calculations* in ``Supercomputing Tools for Science and Engineering'', ed. D. Laforenza and R. Perego, Franco Angeli, Milano, (1990), 645-649.

Publications

1. Hu, Minmin; Linder, Douglas; Buongiorno Nardelli, Marco; Striolo, Alberto, *Hydrogen Adsorption on Platinum–Gold Bimetallic Nanoparticles: A Density Functional Theory Study*, Journal of Physical Chemistry C, *in press*.
2. Pronschinske, Alex; Chen, Yifeng; Lewis, Geoffrey; Calzolari, Arrigo; Shultz, David; Buongiorno Nardelli, Marco; Dougherty, Daniel, *Modification of Molecular Spin Crossover in Ultra-Thin Film*, NanoLetters, **13** (4), 1429–1434 (2013).
3. Xiaodong Li, Jeffrey T. Mullen, Zhenghe Jin, Kostyantyn M. Borysenko, M. Buongiorno Nardelli and Ki Wook Kim, *Intrinsic electrical transport properties of monolayer silicene and MoS2 from first principles*, Phys. Rev. B **87**, 115418 (2013)
4. G. De Marzi, L. Morici, L. Muzzi, A. della Corte and M. Buongiorno Nardelli, *Strain sensitivity and superconducting properties of Nb3Sn from first principles calculations*, J. Phys.: Condens. Matter **25** (2013)
5. Calzolari, Arrigo; Chen, Yifeng; Lewis, Geoffrey; Dougherty, Daniel; Shultz, David; Buongiorno Nardelli, Marco, *Complex Materials for Molecular Spintronics Applications: Cobaltbis(dioxolene) Valence Tautomers, from Molecules to Polymers*, Journal of Physical Chemistry B, **116**(43):13141-8 (2012).
6. Arrigo Calzolari, Thushari Jayasekera, K.W. Kim and Marco Buongiorno Nardelli, *Ab initio thermal transport properties of nanostructures from density functional perturbation theory*, J. Phys.: Condens. Matter **24** (2012) 492204.
7. R. Mao, T. Jayasekera, A. Calzolari, B. D. Kong, K. W. Kim, and M. Buongiorno Nardelli, *Phonon Engineering in Nanostructures: Controlling Interfacial Thermal Resistance in Graphene/Dielectric Heterojunctions*, Applied Physics Letters, **101**, 113111 (2012).

8. Kesong Yang, Wahyu Setyawan, Shidong Wang, Marco Buongiorno Nardelli, and Stefano Curtarolo, *A search model for topological insulators with high-throughput robustness descriptor,* Nature Materials, **11**(7) 614-9 (2012).
9. A.N. Sidorov, D. K. Gaskill, M. Buongiorno Nardelli, J. L. Tedesco, R. L. Myers-Ward, C. R. Eddy Jr., T. Jayasekera, K. W. Kim, R. Jayasingha,A. Sherehiy,R. Stallard,and G. U. Sumanasekera *Charge transfer equilibria in ambient-exposed epitaxial graphene on (000-1) 6H-SiC*, J. of Appl. Phys. 111(11) (2012)..
10. Thushari Jayasekera, K. W. Kim, and M. Buongiorno Nardelli, *Electronic and Structural Properties of Turbostratic Epitaxial Graphene on the 6H-SiC (000-1) Surface*, Proceedings of ICSCRM 2011, *in press*.
11. V. Ranjan, Marco Buongiorno Nardelli, and J. Bernholc, *Electric field induced phase transitions in polymers: A novel mechanism for high speed energy storage*, Phys. Rev. Lett., **108**, 087802 (2012).
12. Andreas Sandin, Thushari Jayasekera, J. E. Rowe, Ki Wook Kim, M. Buongiorno Nardelli, Daniel B. Dougherty, *Multiple coexisting intercalation structures of sodium in epitaxial graphene-SiC interfaces*, Phys. Rev. B, **85***,* 125410 (2012).
13. Stefano Curtarolo, Wahyu Setyawan, Richard H. Taylor, Shidong Wang, Junkai Xue, Kesong Yang, Gus L. W. Hart, Stefano Sanvito, Marco Buongiorno Nardelli, Natalio Mingo, and Ohad Levy *AFLOWLIB.ORG: a distributed materials properties repository from high-throughput ab initio calculations,* Computational Materials Science, **58** 227 (2012).
14. Meng Miao, Ying-Chun Liu, Qi Wang, Tao Wu, Liping Huang, Keith Gubbins, and Marco Buongiorno Nardelli, *Activation of water on the TiO2 (110) surface: the case of Ti adatoms,* Journal of Chemical Physics, **136**, 064703 (2012).
15. X. Li, K. M. Borysenko, J. Mullen, M. Buongiorno Nardelli, K. W. Kim, *Electron transport properties of bilayer graphene*, Phys. Rev. B, **84**, 195453 (2011).
16. Thushari Jayasekera, S. Xu, K. W. Kim, and M. Buongiorno Nardelli, *Electronic properties of the graphene/6H-SiC*$(000\bar{1})$ *interface: A first-principles study*, Phys. Rev. B **84**, 035442 (2011).
17. Morrow, Brian; Resasco, Daniel; Striolo, Alberto; Buongiorno Nardelli, Marco, *CO Adsorption on Noble Metal Clusters: Local-Environment Effects*, Journal of Physical Chemistry, C, **115**, 5637 (2011).
18. K. M. Borysenko, J. T. Mullen, X. Li, Y. G. Semenov, J. M. Zavada, M. Buongiorno Nardelli, and K. W. Kim, *Electron-phonon interactions in bilayer graphene*, Phys. Rev. B **83**, 161402(R) (2011) [Editors' suggestion]
19. S. Paul and M. Buongiorno Nardelli, *Rational computational design of optimal catalytic surfaces*, Appl. Phys. Lett. **97**, 233108 (2010)
20. X. Li, E. A. Barry, J. M. Zavada, M. Buongiorno Nardelli, K. W. Kim, *Surface Polar Phonon Dominated Electron Transport in Graphene*, Appl. Phys. Lett. **97**, 232105 (2010).
21. Y. Chen, T. Jayasekera, A. Calzolari, K.W. Kim and M. Buongiorno Nardelli, *Thermoelectric properties of graphene nanoribbons, junctions and superlattics*, J. of Physics: Condensed Matter, Fast Track Communication, **22,** 372202 (2010) [Selected as one of the **Highlights of 2010**].

22. X. Li, E. A. Barry, J. M. Zavada, M. Buongiorno Nardelli, K. W. Kim, *Influence of Carrier-Carrier Scattering on Electron Transport in Monolayer Graphene*, Appl. Phys. Lett. **97**, 082101 (2010), also arXiv:1005.2631.
23. V. Ranjan, L. Yu, Serge Nakhmanson, Jerry Bernholc and M. Buongiorno Nardelli, *Polarization effects and phase equilibria in high-energy-density polyvinylidene-fluoride-based polymers*, Acta Cryst. A **66**, 553–557 (2010).
24. Yingchun Liu, Liping Huang, Keith Gubbins, and Marco Buongiorno Nardelli, *Dissociation of Water over Ti-Decorated C_{60}*, J. Chem. Phys. **133**, 084510 (2010).
25. Santagata, Nancy; Lakhani, Amit; Davis, Bryce; Luo, Pengshun; Buongiorno Nardelli, Marco; Pearl, Thomas, *Chiral Steering of Molecular Organization in the Limit of Weak Adsorbate-Substrate Interactions: Enantiopure and Racemic Tartaric Acid Domains on Ag(111)*, The Journal of Physical Chemistry C (2010) **114** (19) pp. 8917-8925
26. Thushari Jayasekera, B. D. Kong, K. W. Kim, and M. Buongiorno Nardelli, *Band Engineering and Magnetic Doping of Epitaxial Graphene on SiC (0001)*, Phys. Rev. Lett. **104**, 146801 (2010).
27. K. M. Borysenko, J. T. Mullen, E. A. Barry, S. Paul, Y. G. Semenov, J. M. Zavada, M. Buongiorno Nardelli and K. W. Kim, *First Principles Analysis of Electron-Phonon Interaction in Graphene*, Phys. Rev. B Rapid Communications, **81**, 121412 (2010).
28. Liping Huang, Ying-Chun Liu, Keith E. Gubbins and Marco Buongiorno Nardelli, *Ti-decorated C60 as catalyst for hydrogen generation and storage*, Applied Physics Letters **96**(6): 063111-063113 (2010).
29. Arrigo Calzolari, Wei Jin, Janice E. Reutt-Robey and Marco Buongiorno Nardelli,*Substrate-Mediated Intermolecular Hybridization in Binary Phthalocyanine Superstructures*, Journal of Physical Chemistry C **114**(2): 1041-1045 (2010).
30. Liping Yu, V. Ranjan, M.Buongiorno Nardelli, J. Bernholc, *First-principles investigations of the dielectric properties of polypropylene/metal-oxide interfaces*, Phys. Rev. B **80**, 165432 (2009).
31. Sujata Paul, Erik E. Santiso and Marco Buongiorno Nardelli, *Sequestration and selective oxidation of carbon monoxide on graphene edges*, Journal of Physics: Condensed Matter, **21**, 355008 (2009).
32. Pantano, A. and M. Buongiorno Nardelli, *Simulation of the Electromechanical Behavior of Multiwall Carbon Nanotubes*, Acs Nano 3(10): 3266-3272 (2009).
33. B.D. Kong, S. Paul, M.Buongiorno Nardelli, K.W. Kim, *First-principles analysis of lattice thermal conductivity in monolayer and bilayer graphene*, Phys. Rev. B, **80**, 033406 (2009).
34. L. Huang, D. Rocca, S. Baroni, K. Gubbins, and M. Buongiorno Nardelli, *Molecular design of photoactive acenes for organic photovoltaics*, J. Chem. Phys., **130**, 194701 (2009).
35. M. Nunez and M. Buongiorno Nardelli, *Onset of ferrielectricity and the hidden nature of nanoscale polarization in ferroelectric thin films,* Phys. Rev. Lett, **101**, 107603 (2008).
36. M. Nunez and M. Buongiorno Nardelli, *Interface phase and tuning of polarization in metal-ferroelectric junctions: A theoretical study*, Appl. Phys. Lett. **92**, 252903 (2008).
37. Liping Yu, V. Ranjan, W. Lu, J. Bernholc, and M. Buongiorno Nardelli, *Equivalence of dipole correction and Coulomb cutoff techniques in supercell calculations*, Phys. Rev. B **77**, 245102 (2008).

38. L. Huang, E.E. Santiso, M. Buongiorno Nardelli and K.E. Gubbins, *Catalytic role of carbons in the methane decomposition for CO and CO_2-free hydrogen generation* J. of Chemical Physics, **128** (21), 214702 (2008).
39. EE Santiso, M Buongiorno Nardelli, KE Gubbins, *Isomerization kinetics of small hydrocarbons in confinement,* Adsorption, **14**, 181 (2008)
40. EE Santiso, M Buongiorno Nardelli, KE Gubbins, *A remarkable shape-catalytic effect of confinement on the rotational isomerization of small hydrocarbons*, JOURNAL OF CHEMICAL PHYSICS, **128** (3): Art. No. 034704 JAN 21 2008
41. G Kim, SC Wang, WC Lu, M Buongiorno Nardelli, J Bernholc, *Effects of end group functionalization and level alignment on electron transport in molecular devices*, JOURNAL OF CHEMICAL PHYSICS, **128** (2): Art. No. 024708 JAN 14 2008
42. A. Calzolari, A. Ferretti and M. Buongiorno Nardelli, *Ab initio correlation effects on the electronic and transport properties of metal(II)-phthalocyanine based devices*, Nanotechnology, **18**, 424013 (2007).
43. S. Wippermann, W.G. Schmidt, A. Calzolari, M. Buongiorno Nardelli, A.A. Stekolnikov, K. Seino, F. Bechstedt, *Quantum conductance of In nanowires on Si(111) from first principles calculations*, Surf. Sci. **601**, 4045 (2007)
44. V. Ranjan, L. Yu, M. Buongiorno Nardelli and J. Bernholc, *Phase Equilibria in High Energy Density PVDF-Based Polymers*, Phys. Rev. Lett., **99**, 047801 (2007).
45. A. Stekolnikov, K. Seino, and F. Bechstedt, S. Wippermann and W. G. Schmidt, A. Calzolari and M. Buongiorno Nardelli, *Hexagon versus Trimer Formation in In Nanowires on Si(111): Energetics and Quantum Conductance*, Phys. Rev. Lett. **98**, 026105 (2007).
46. Santiso EE, Kostov MK, George AM, Buongiorno Nardelli M, Gubbins KE, *Confinement effects on chemical reactions - Toward an integrated rational catalyst design* Appl. Surf. Sci. **253**, 5570-5579 (2007)
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Congresses

Invited talks at Conferences

1. "GPU computing in electronic-structure calculations: accelerating quantum-ESPRESSO and WanT to hybrid architectures", Invited, ORNL
2. "First Principles Methods and Hydraulic Fracturing: Challenges and Future Perspectives", Invited, NSF
3. "Quantum-ESPRESSO Summer School", Lecturer, Penn State University
4. "Novel paradigms for molecular spintronics: valence tautomeric complexes and graphene functionalizations" Invited, University College, TYC
5. "Science of Music, Music of Science", Invited, Imperial College
6. "First Principles Theory of Charge Mobility and Heat Transport in Graphene-based Systems". Invited, Imperial College
7. "First principles design of advanced materials for energy applications", Invited, "Fundamental Issues at the Interface of Materials and Mechanics Related to Energy Applications" (FIMMEA-2012)
8. "Theory of the electronic and transport properties of epitaxial graphene", "Specialists Meeting on Carbon", Puerto Vallarta, Jalisco, Mexico, 26th - 30th September 2011.
9. "Recent advances in molecular electronics and spintronics from first principles", IV International Conference on Surfaces, Materials and Vacuum", Puerto Vallarta, Jalisco, Mexico, 26th - 30th September 2011.
10. "Recent advances in molecular electronics and spintronics from first principles", "Materials by Design" workshop, Oak Ridge National Laboratory, Oak Ridge, TN, September 21, 2011.
11. "First principles calculations of charge mobility and heat transport in graphene-based systems", CNMS Users Meeting, Oak Ridge National Laboratory, Oak Ridge, TN, September 19, 2011.
12. "Electronic and thermal transport in nanostructures", CECAM workshop on "Thermal and electronic transport", Lugano (Switzerland) from June 20th to 22nd, 2011.
13. "Theory of the electronic and transport properties of epitaxial graphene", APS March Meeting 2011.
14. "Recent advances in molecular spintronics from first principles", XIX International Materials Research Congress, Cancún, México, August 14-18, 2010
15. "First principles calculations of charge mobility and heat transport: a practical tool-set for the efficient design of novel materials and devices for nanoelectronic applications", XVIII International Materials Research Congress, Cancún, México, August 18-22, 2009
16. "Carbon Nanostructures for Energy and Environmental Applications", 14th Canadian Semiconductor Technology Conference, Hamilton, Ontario, Canada, August 10-14, 2009.
17. "Polarization Effects and Phase Equilibria in High Energy Density PVDF-Based Polymers", CECAM workshop on "Structural Transitions in Solids: Theory, Simulations, Experiments and Visualization Techniques", Lugano, Switzerland, July 8-11, 2009
18. "Carbon Nanostructures for Energy and Environmental Applications", CECAM workshop on "Modeling of Carbon and Inorganic Nanotubes and Nanostructures", Lusanne, Switzerland, May 13-15, 2009.

19. “Carbon Nanostructures for Energy and Environmental Applications”, XVII International Materials Research Congress, Cancún, México, August 17-21, 2008
20. "Geometrical phases and the Coulomb buffer in nanoscale interfaces", XVI International Materials Research Congress, Cancún, México, August 19-24, 2007
21. "Wannier Functions and Quantum Transport in Nanostructures", CECAM-psi_k workshop “Maximally Localized Wannier Functions: Concepts, Applications, and Beyond", 27-29 June, 2007, Lyon, France.
22. “Novel advances in the Physics and Chemistry of Carbon Nanotubes”, CECAM-psi_k workshop “Simulations of Novel Carbon Materials”, 25-28 October 2006, Lyon, France
23. “Electronic transport in nanostructures from first principles”, XV International Materials Research Congress, Cancún, México, August 20-24, 2006
24. “Novel advances in the Physics and Chemistry of Carbon Nanotubes”, Workshop on “Electronic Structure Methods and their Applications, 10-22 July 2006, Bangalore, India
25. “Iterative solutions of the electronic structure problem”, Workshop on “Electronic Structure Methods and their Applications, 10-22 July 2006, Bangalore, India
26. “Interface phases and the Schottky-Mott theory revisited “, 33rd Conference on the Physics and Chemistry of Semiconductor Interfaces (PCSI-33), January 15-19, 2006, in Cocoa Beach, FL.
27. “Interface phases and the Schottky-Mott theory revisited “, ITAMIT Workshop on Computational Materials and Electronics, Austin Texas, October 20-22, 2005.
28. “Crystalline Oxides on Silicon: a future for the nanotransistor”, March Meeting of the APS, Los Angeles, CA, March 2005.
29. “The interface phase and the Schottky barrier at a crystalline dielectric on Silicon”, IUVSTA 2004, Venice, June 2004.
30. “The interface phase and the Schottky barrier at a crystalline dielectric on Silicon”, 5th MOTOROLA workshop on Computational Materials and Electronics, Austin, TX, November 13-14, 2003.
31. “Crystalline Oxides on Semiconductors: a future for the nanotransistor”, SESAPS meeting, Wilmington, NC, November 8-10, 2003.
32. “The interface phase and the Schottky barrier for a crystalline dielectric on Silicon”,, International Conference on Advanced Materials (IUMRS-ICAM2003), Yokohama, Japan, October 8-10, 2003.
33. `` Quantum transport in nanotube-based structures’’, Workshop on “Quantum Phases at the Nanoscale”, Centro Ettore Majorana, Erice, Italy, July 15-20, 2002.
34. `` Polarization effects in nanotube structures’’, 5th International School on the Applications of Surface Science Techniques, Centro Ettore Majorana, Erice, Italy, July 15-20, 2002.
35. ``Ab initio quantum transport calculations: application to nanostructures’’, INFM annual meeting 2002, Bari, Italy, June 24-28, 2002.
36. ``Polarization effects in nanotubolar structures’’, Electronic Structure workshop, Berkeley, CA, June 6-8, 2002.
37. ``Quantum transport in nanotube-based structures", MRS fall meeting, Boston, November 26-30, 2001.
38. ``Electronic and transport properties of carbon nanostructures", Towards Molecular Electronics, TME’01, Šrem, Poland, June 25-30, 2001.

39. "Quantum Transport in Nanotube-Based Structures", Mardi Gras Conference on Multiscale Simulation, Theoretical, and Experimental Approaches to Deformation, Friction, Fatigue, and Fracture, Baton Rouge, Louisiana, February 2001.
40. ``Electronic and transport properties of carbon nanotubes", Psi-k Conference, Schwabisch Gmund, Germany, August 22-26, 2000.
41. ``Mechanical deformations and electronic transport in carbon nanotubes", MRS Spring Meeting, San Francisco, April 24-28, 2000.
42. ``Theory of electronic and transport properties of carbon nanotubes", APS March Meeting, Minneapolis, Indiana, March 2000.
43. ``Mechanical and transport properties of carbon nanotubes", ``Fullerenes 99" workshop, Aug. 29-Sep. 2, 1999, Chateau de Bonas, France.
44. ``Electronic transport in nanostructures: application to carbon nanotubes", workshop on ``New methods in electronic structure", May 21-24, 1999, Urbana, IL.
45. ``Brittle and ductile behaviour in carbon nanotubes", 9th ``International Workshop on Computational Materials Science: Electronic Structure Theory and Simulations", 14-16 January 1999, Trieste, Italy.
46. ``Growth and mechanical properties of Carbon Nanotubes", MRS Fall Meeting, Boston, November 30-December 4, 1998.
47. ``Wide-gap nitrides: from growth morphology to device behavior", M. Buongiorno Nardelli, K. Rapcewicz, C. Bungaro, E.L. Briggs and J. Bernholc, APS March Meeting, Los Angeles, California, March 1998.
48. ``Theory of Surfaces, Adsorbates, Heterostructures, Defects and Ordering in Nitride Semiconductors", J. Bernholc, P. Boguslawski, C. Bungaro, M. Buongiorno Nardelli and K. Rapcewicz, International GaN Workshop at Schloss Ringberg, ``Surface Morphology, Interfaces and Growth of the III-Nitrides", Schloss Ringberg, Germany, January 20 - 24 1998.
49. ``Theory of Surfaces and Interfaces in Wide-Gap Nitrides." M. Buongiorno Nardelli, K. Rapcewicz and J. Bernholc, Electronic Structure 1997 Workshop, Cornell University, Ithaca, New York, May 1997.
50. ``Theory of Growth and Mechanical Properties of Carbon Nanotubes." J. Bernholc, C. J. Brabec, M. Buongiorno Nardelli, M.-P. Campbell, A. Maiti, K. Rapcewicz, C. Roland, and B. I. Yakobson, Carbon Nanotube Workshop, Rice University, Houston, Texas, May 1997.
51. ``Theory of Surfaces and Interfaces in Wide-Gap Nitrides." K. Rapcewicz, M. Buongiorno Nardelli and J. Bernholc, APS March Meeting, Kansas City, Missouri, March 1997.
52. ``Real-Space Multigrid Calculations for Surfaces, Interfaces, and Proteins." J. Bernholc, C. Brabec, E.L. Briggs, M. Buongiorno Nardelli, K. Rapcewicz, C. Roland, M. Wensell, APS March Meeting, Kansas City, Missouri, March 1997.
53. ``Theory of Surface Reconstructions in GaN." M. Buongiorno Nardelli, K. Rapcewicz and J. Bernholc, Workshop on ``Wide Band Gap Semiconductors: Defects and Fundamental Parameters", Research Triangle Park, NC, January 1997.
54. ``DFT Simulations Using a Real Space Grid." J. Bernholc, C. Brabec, E.L. Briggs, M. Buongiorno Nardelli, K. Rapcewicz, C. Roland, D.J. Sullivan, and M. Wensell, 8th International Workshop on Computational Condensed Matter Physics: Total Energy and Force Methods, Trieste, Italy, January 1997.

55. ``Theory of Surfaces and Interfaces in Wide-Gap Nitrides." K. Rapcewicz, M. Buongiorno Nardelli and J. Bernholc, 1st Symposium on III-V Nitrides: Materials and Device Processing held at the 189th Electrochemical Society Meeting, May 1996.
56. ``Theory of Native Defects, Surfaces and Interfaces of GaN, AlN, and SiC." J. Bernholc, P. Boguslawski, E.L. Briggs, M. Buongiorno Nardelli, B. Chen, K. Rapcewicz, and Z. Zhang, MRS Spring Meeting, San Francisco, California, April 1996.
57. ``Theory of Nitrides." J. Bernholc, P. Boguslawski, E.L. Briggs, M. Buongiorno Nardelli, B. Chen, K. Rapcewicz, B. Yakobson, and Z. Zhang, 3rd Workshop on Wide-Bandgap Nitrides, St. Louis, Missouri, March 1996.
58. ``Phonon softening and low symmetry phases of Cesium Iodide." 6th International Workshop on Computational Condensed Matter Physics, Trieste, 11-13 January 1993.
59. ``Two-Grid algorithm for fast convergence in self-consistent electronic structure calculations.", round table on Minimization Strategies in Computer Simulations, Trieste, Italy, 16 March 1993.
60. ``Hydrogen adsorption on GaAs and Si cleavage surfaces.", CECAM (Centre Europeen de Calcul Atomique et Moleculaire) workshop on ``Electronic Structure of Surface Systems", Paris, France, 22-31 October 1990.
61. ``Hydrogen adsorption on compound semiconductor surfaces", 14th Annual Meeting on ``Advances in surfaces and interfaces physics", Modena, Italy, December 1989.

Seminars and Colloquia

1. TBA, Zhejiang University, Hangzhou, China, Spring 2012.
2. "A Soiree on Theory and Simulation of Spintronic Materials", London Centre for Theory and Simulation of Materials, Imperial College, London, GB, January 23, 2012.
3. “Computational design of materials for the 21st century”, North Texas University and CASCaM, April 28, 2011.
4. “Computational design of materials for the 21st century”, Penn State University, January 13, 2011.
5. “Computational design of materials for the 21st century”, Zhejiang University, Hangzhou, China, October 18, 2010.
6. “Physics at nanoscale: Theoretical and Computational Aspects”, ICTP school, Hanoi, VietNam, December 2009.
7. “Carbon Nanostructures for Energy and Environmental Applications”, Max-Planck Institute for Chemical Physics of Solids, Dresden, Germany, July 6, 2009.
8. "Geometrical phases and the Coulomb buffer in nanoscale interfaces", Argonne National Laboratory, Argonne, Il, April 17, 2008
9. "Geometrical phases and the Coulomb buffer in nanoscale interfaces", Yale University, New Haven, CN, June 2007.
10. “First principles calculations of quantum transport in nanostructures”, Central Michigan University, Mt. Pleasant, MI, 23 Sep. 2004.
11. “Crystalline oxides on semiconductors: a future for the nanotransistor”, ELETTRA Sincrotrone Trieste, Trieste, Italy, 29 June 2004.

12. “Crystalline oxides on semiconductors: a future for the nanotransistor”, Universita’ di Modena, Modena, Italy, 22 June 2004.
13. “Crystalline oxides on semiconductors: a future for the nanotransistor”, Wake Forest University, Wiston-Salem, NC, April 15, 2004.
14. “Ab initio quantum transport calculations: application to nanostructures”, ENEA “ La Casaccia” research laboratory, December 2003.
15. ``Ab initio quantum transport calculations: application to nanostructures’’, Universita’ di Roma “ Tor Vergata”, Roma, Italy, July 11, 2002.
16. ``Polarization effects in nanotubolar structures’’, Universita’ di Modena, Modena, Italy, June 19, 2002.
17. ``Theory of electronic transport in carbon nanotubes’’, Universita’ di Modena, Modena, Italy, October 3, 2001.
18. ``Carbon nanotubes: a theoretical laboratory", Fall Colloquium, University of Louisville, Louisville, Kentucky, November 5, 1999.
19. ``Mechanical and transport properties of carbon nanotubes", Sep 4, 1999, Univ. Paris VI, France.
20. ``Theory of surfaces and interfaces in wide-gap nitrides", Joint ICTP/SISSA seminar, Trieste, Italy, 8 August 1997.
21. ``Recent advances in large-scale computer simulations: from atomic to nanostructure physics." Dep. of Physics, III Univ. of Rome, Rome, Italy, 18 July 1997.
22. ``Recent advances in large-scale computer simulations: from atomic to nanostructure physics." Dep. of Physics, Univ. of Modena, Modena, Italy, 23 July 1997.
23. ``New developments in atom-surface scattering theory", University of Nottingham, Nottingham, UK, 15 November 1994.
24. ``Ab-initio lattice dynamics from density functional methods: theory and applications", Universite' de Marne-la-Vallee, Paris, France, 30 June 1994.
25. ``Introduction to Density Functional Theory electronic structure calculations and applications to semiconductor surfaces", AREA di Ricerca di Trieste, Italy, 13 January 1993.

Invited talks at Conferences, presented by a co-author

1. "Multiscale Simulations and Design of Nanomaterials and Devices," keynote lecture, J. Bernholc, J. Jiang, V. Ranjan, F. Ribeiro, M. Hodak, X. Zheng, W. Lu, V. Meunier, M. Buongiorno Nardelli, L. Yu, CECAM Workshop on Computational Approaches to Semiconductor, Carbon and Magnetic Nanostructures, Lyon, France, June 2008.
2. "First-principles simulations of failure mechanisms, mechanical strength and electrome-chanical response," J. Bernholc, M. Buongiorno Nardelli, W. Lu, S. Wang and Q. Zhao, APS March Meeting, Denver, CO, 2007.
3. “Atomic Scale Design of Nanostructures,” J. Bernholc, W. Lu, S. Nakhmanson, M. Buongiorno Nardelli, G. Kim, V. Meunier, F. Ribeiro, P. Hahn, W. G. Schmidt, S. Wang, and Q. Zhao, Spring American Chemical Society Meeting, Chicago, Illinois, March 2007.

4. “Atomic Scale Design of Nanostructures,” J. Bernholc, W. Lu, S. Nakhmanson, M. Buongiorno Nardelli, G. Kim, V. Meunier, F. Ribeiro, P. Hahn, W. G. Schmidt, S. Wang, and Q. Zhao, Spring MRS Meeting, San Francisco, California, April 2007.
5. "Real-Space Electronic Structure Method with Multigrid Acceleration (RMG)," J. Bernholc, W. Lu, Q. Zhao, F. Ribeiro, S. Wang, M. Hodak, P. Hahn, M. Buongiorno Nardelli, V. Meunier, and G. Schmidt, International Symposium on Theory of Atomic and Molecu-lar Clusters TAMC 5, Richmond, Virginia, May 2007.
6. “Design of new ferroelectric polymers through computer simulation”, S. Nakhmanson, M. Buongiorno Nardelli and J. Bernholc, Sixteenth Annual Workshop on Recent Developments in Electronic Structure Methods (ES2004), Rutgers, May 2004.
7. “Mechanical and Polarization Properties of Nanostructures," J. Bernholc, M. Buongiorno Nardelli, V. Meunier, S. Nakhmanson, and Q. Zhang, 3rd International Conference on Computational Modeling and Simulation of Materials, Special Symposium “Modeling and Simulating Materials Nanoworld,” Acireale (CT), Sicily, Italy, June 2004.
8. “Simulations of nanotube-based structures and devices," J. Bernholc, M. Buongiorno Nardelli, W. Lu, V. Meunier, S. Nakhmanson and Q. Zhao, Conference on Foundations of Nanoscience: Self-assembled Architectures and Devices," Snowbird, Utah, April 2004.
9. “Theory and simulations of nanotubes, nanowires and ferroelectric polymers," J. Bernholc, M. Buongiorno Nardelli, W. Lu, V. Meunier, S. Nakhmanson, W. G. Schmidt, S. Wang and Q. Zhao, MRS Spring Meeting, San Francisco, April 2004.
10. “Theory and simulations of nanotubes, nanowires and ferroelectric polymers," J. Bernholc, M. Buongiorno Nardelli, W. Lu, V. Meunier, S. Nakhmanson, W. G. Schmidt, S. Wang and Q. Zhao, Indo-US workshop on Nanoscale materials: From Science to Technology, Puri, India, April 2004.
11. “Theory and simulations of nanotubes, nanowires and complex surface structures, J. Bernholc, M. Buongiorno Nardelli, W. Lu, V. Meunier, W. G. Schmidt, S. Wang and Q. Zhao, 12th Mardigras Conference on Materials and Modeling for Information Technology, Baton Rouge, LA, February 2004.
12. “Superpolar polymers by design”, S. Nakhmanson,M. Buongiorno Nardelli, J. Bernholc, Workshop on Fundamental Physics of Ferroelectrics, Williamsburg, VA, February 2004.
13. “New piezoelectric and pyroelectric materials by first principles design”, Center for Computational Materials Science, Naval Research Lab, Washington, DC, October 2003.
14. “DFT-optimized localized orbitals and nearly O(N) calculations of quantum transport," J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, W. Lu, and Q. Zhao, CECAM-ESF/Psi-k Workshop on Electronic Transport in Molecular Systems, Lyon, France, June 2003.
15. “Quantum Transport Theory in Carbon Nanostructures,” V. Meunier, W. Shelton, T. Zacharia, J.-C. Charlier, C. Roland, J. Bernholc, M. Buongiorno Nardelli, 2003 MRS Spring Meeting, San Francisco, California, April 2003.
16. “Large-Scale Multigrid Simulations of Novel Materials and Nanoscale Devices," J. Bernholc, E. L. Briggs, M. Buongiorno Nardelli, J.-L. Fattebert, W. Lu, V. Meunier, S. Nakhmanson, W. G. Schmidt, and Q. Zhao, 225th ACS National Meeting, New Orleans, Louisiana, March 2003
17. “Designing novel polar materials through computer simulations,” S. Nakhmanson, M. Buongiorno-Nardelli and J. Bernholc, Mardi Gras Physics Conference, Louisiana State University, Baton Rouge, LA, February 2003.

18. “Atomic Transformations, Electronic Properties And Quantum Transport In Nanotubes, J. Bernholc, M. Buongiorno Nardelli," V. Meunier, S. Nakhmanson, C. Roland and Q. Zhao, 54th Southeast Regional Meeting of the American Chemical Society, Charleston, South Carolina, November 2002.
19. “Polarization effects in nanotube structures," M. Buongiorno Nardelli, J. Bernholc, A. Calzolari, N. Marzari, V. Meunier, S. Nakhmanson, C. Roland, I. Souza, Fourteenth Annual Workshop on Recent Developments in Electronic Structure Algorithms, Berkeley, California, June 2002.
20. “Electronic, Structural, and Transport Properties of Nanotubes," J. Bernholc, M. Buongiorno Nardelli, V. Meunier, S. Nakhmanson, C. Roland, and Q. Zhao, Workshop on Computational Nanotechnology: Industrial Relevance and Applications, Washington, DC, May 2002.
21. “Quantum mechanics on the nanoscale: from electronic structure to virtual materials," J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, V. Meunier, S. Nakhmanson, C. Roland, W. G. Schmidt, and Q. Zhao, DOE Workshop on Theory and Modeling in Nanoscience, San Francisco, California, May 2002.
22. “Mechanical Transformations, Strength, Pyroelectricity, and Electron Transport in Nanotubes," J. Bernholc, M. Buongiorno Nardelli, V. Meunier, S. Nakhmanson, D. Orlikowski, C. Roland and Q. Zhao, 2002 International Conference on Computational Nanoscience and Nanotechnology, San Juan, Puerto Rico, April 2002
23. “Multigrid DFT calculations, optimized localized orbitals and nearly *O(N)* calculations of quantum transport," J. Bernholc, E. L. Briggs, M. Buongiorno Nardelli, J.-L. Fattebert, W. Lu, V. Meunier, S. Nakhmanson, W. G. Schmidt, and Q. Zhao, Workshop on Linear Scaling Electronic Structure Methods, Institute for Pure and Applied Mathematics, University of California Los Angeles, April 2002.
24. “Quantum transport in nanotube-based structures," M. Buongiorno Nardelli, J.-L. Fattebert and J. Bernholc, MRS Fall Meeting, Boston, November 2001.
25. “Atomic Transformations, Electronic Properties and Quantum Transport in Nanotubes," J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, V. Meunier, C. Roland and Q. Zhao, 68th Annual Meeting of the Southeastern Section of the APS, Charlottesville, Virginia, November 2001
26. “Nanotube Electronic and Transport Properties," J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, D. Orlikowski, C. Roland and Q. Zhao, IUVSTA 15th International Vacuum Congress, San Francisco, October 2001
27. “Grid-optimized localized orbitals and nearly O(N) ab initio calculations of quantum conductance," J. Bernholc, M. Buongiorno Nardelli, and J.-L. Fattebert, CECAM Workshop on local orbitals and linear-scaling ab initio calculations, Lyon, France, September 2001.
28. “Theoretical investigations of quantum transport, pyroelectric effects and Li intercalation in nanotubes," J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, V. Meunier, C. Roland, and Q. Zhao, Workshop on Nanotechnology in Carbon and Related Materials, Brighton, United Kingdom, September 2001.
29. "Atomic transformations, strength, plasticity and electron transport in carbon nanotubes," J. Bernholc, M. Buongiorno Nardelli, V. Meunier, D. Orlikowski, C. Roland and Q. Zhao,

Symposium on Modeling and Simulation of Micro and Nano Systems, 6th U.S. National Congress on Computational Mechanics, Dearborn, Michigan, August 2001.

30. "Theoretical studies of quantum transport, pyro- and piezo-electric effects and lithium intercalation," J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, V. Meunier, C. Roland, and Q. Zhao, International Workshop on the Science and Application of Nanotubes 'Nanotubes 01', Potsdam, Germany, July 2001.
31. "Theoretical Studies of Carbon Nanotubes: Atomic Deformations and Quantum Transport," J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, V. Meunier, D. Orlikowski, C. Roland, and Q. Zhao, APS March Meeting, Seattle, March 2001.
32. ``Nanotube Electronic and Transport Properties," J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, D. Orlikowski, C. Roland and Q. Zhao, IUVSTA 15th International Vacuum Congress, San Francisco, October 2001.
33. ``Atomic transformations, strength, plasticity and electron transport in strained carbon nanotubes," J. Bernholc, M. Buongiorno Nardelli, D. Orlikowski, C. Roland and Q. Zhao, Workshop on Fiber Fracture, Palma de Mallorca, Spain, October 2000.
34. ``Multigrid methods in ab initio simulations of materials," J. Bernholc, E. L. Briggs, M. Buongiorno Nardelli, J.-L. Fattebert, W. G. Schmidt, Q. Zhao, and F. Bechstedt, 3rd SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, Pennsylvania, May 2000.
35. ``Massively Parallel Ab Initio Simulations for Surfaces and Nanotubes," J. Bernholc, E. L. Briggs, M. Buongiorno Nardelli, J.-L. Fattebert, D. Orlikowski, C. Roland, W. G. Schmidt, Q. Zhao, and F. Bechstedt, Mardi Gras Conference on Materials Design: Experimental and Computational Challenges, Baton Rouge, Louisiana, March 2000.
36. ``Ab initio simulations of semiconductors and fullerenes," J. Bernholc, E. L. Briggs, M. Buongiorno Nardelli, J.-L. Fattebert, D. Orlikowski, C. Roland, W. G. Schmidt, Q. Zhao, and F. Bechstedt, workshop entitled "Fifteen years of the Car-Parrinello method in Physics and Chemistry," Minneapolis, Minnesota, March 2000.
37. ``Theory of carbon nanotube devices", C. Roland, J. Bernholc, M. Buongiorno Nardelli, H. Guo, H. Mehrez, D. Orlikowski, J. Taylor, J. Wang and Y. Wei; Joint US-JAPAN Meeting on Surfaces and Mesoscopic Phenomena; Park City, Utah, April 2000.
38. ``Theoretical investigations of carbon nanotubes: mechanical and electronic properties", C. Roland, J. Bernholc, M. Buongiorno Nardelli, D. Orlikowski, and Q. Zhao; Nasa Microgravity Conference, Huntsville, Al, June 2000.
39. ``Atomic transformations and quantum transport in carbon nanotubes", J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, D. Orlikowski, R. Roland and Q. Zhao, MRS Fall Meeting, Boston, December 1999.
40. ``Atomic transformations and quantum transport in carbon nanotubes", J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, D. Orlikowski, C. Roland and Q. Zhao, Workshop on Nanotechnology in Carbon and Related Materials, Brighton, United Kingdom, September 1999.
41. ``Mechanical Properties and Electronic Transport in Carbon Nanotubes", J. Bernholc, M. Buongiorno Nardelli, J.-L. Fattebert, D. Orlikowski, R. Roland and Q. Zhao, ``Nanotubes 99. International workshop on the science and applications of nanotubes", East Lansing, Michigan, July 1999.

42. ``Theoretical investigations of carbon nanotubes: Growth, Quantum Dots and STM Images", C. Roland, J. Bernholc, M. Buongiorno Nardelli, and D. Orlikowski, 1999 Beijing Workshop on Transport and Mesoscopic Systems, Beijing, China, July 1999.
43. ``Theoretical investigations of carbon nanotubes: growth, quantum dots and STM images", C. Roland, J. Bernholc, M. Buongiorno Nardelli, C. Brabec, A. Maiti and D. Orlikowski, Molecular Simulations Web-based Conference, sponsored by Vei Inc, May, 1999.
44. ``Large-scale simulations and design of nanoscale materials and devices: structural, mechanical and electrical properties of nanotubes", J. Bernholc, E.L. Briggs, M. Buongiorno Nardelli, J.-L. Fattebert, D. Orlikowski, and C. Roland, Engineering Foundation Conference on Nanocomposite Materials: Design and Applications, Girdwood, Alaska, March 1999.
45. ``Theory of growth and mechanical properties of nanotubes", J.Bernholc, M. Buongiorno Nardelli, C. Roland and B. Yakobson, APS March meeting, Atlanta, Georgia, March 1999.
46. ``Kinetics and Growth of Diverse Material Systems: Si (100) step flow and carbon nanotubes", C. Roland, J. Bernholc, C. Brabec, E.L. Briggs, M. Buongiorno Nardelli, A. Maiti and M.G. Wensell, Research School on Computational Methods in Condensed Matter Physics, Sjoekulla Finland, October 1998.
47. ``Growth of carbon nanotubes", C. Roland, J. Bernholc, C. Brabec, M. Buongiorno Nardelli, and A. Maiti, CECAM Workshop on {\it Surfaces and Interfaces Far From Equilibrium}, Lyon France, July 1998.
48. ``Growth and Mechanical Properties of Carbon Nanotubes", J. Bernholc, C. Brabec, M. Buongiorno Nardelli, A. Maiti, C. Roland and B.I. Yakobson, CECAM Workshop on {\it Carbon Nanotubes}, Lyon France, September 1998.
49. ``Real-Space multigrid calculations for surfaces, nanotubes and proteins", J. Bernholc, E.L. Briggs, C. Bungaro, M. Buongiorno Nardelli, M. Ramamoorthy, K. Rapcewicz, C. Roland, M.G. Wensell, B.I. Yakobson, C.J.Brabec and D.J. Sullivan, Symposium on Atomic-Level Simulation of Materials: New Methods and novel applications, Annual ASM/TMS meeting, San Antonio, Texas, February 1998.
50. ``Growth, Closure, and Breakage Mechanisms of Nanotubes", J. Bernholc, M. Buongiorno Nardelli, C. J. Brabec, A. Maiti, C. Roland, and B. I. Yakobson, Tenth annual workshop on Recent Developments in Electronic Structure Algorithms, Philadelphia, Pennsilvania, May 1998.
51. ``Real-Space multigrid calculations for surfaces, nanotubes and proteins", J. Bernholc, E.L. Briggs, C. Bungaro, M. Buongiorno Nardelli, M. Ramamoorthy, K. Rapcewicz, C. Roland, M.G. Wensell, B.I. Yakobson, C.J.Brabec and D.J. Sullivan, Workshop on computational material physics in the southeast, Nashville, Tennessee, November 1997.
52. ``Theory of native defects, surfaces and interfaces of GaN, Al,N and SiC", J. Bernholc, P. Boguslawsky, E.L. Briggs, M. Buongiorno Nardelli, B. Chen, K. Rapcewicz and Z. Zhang, MRS Spring Meeting, San Francisco, California, April 1996.
53. ``Theory of Nitrides", J. Bernholc, P. Boguslawsky, E.L. Briggs, M. Buongiorno Nardelli, B. Chen, K. Rapcewicz, B. Yakobson and Z. Zhang, Third workshop on wide-gap nitrides, St.Louis, Missuri, March 1996.

Contributed talks at Conferences

1. “Effects of Electron-Phonon Interaction in Graphene: The First Principle Calculation”, APS March Meeting 2010, March 15–19, 2010; Portland, Oregon
2. “Modification of interfacial electronic structure as a function of organic overlayer stereochemistry”, APS March Meeting 2010, March 15–19, 2010; Portland, Oregon
3. “First principles study of the activation of carbon dioxide on catalytic surfaces”, APS March Meeting 2010, March 15–19, 2010; Portland, Oregon
4. “First principles calculations of thermal phonon transport in nanostructures”, APS March Meeting 2010, March 15–19, 2010; Portland, Oregon
5. “Thermal transport in graphitic nanostructures: Analytic force constants and first principles calculations”, APS March Meeting 2010, March 15–19, 2010; Portland, Oregon
6. “First Principles Study of Phase Transformations in Polyvinylidene Fluoride”, APS March Meeting 2010, March 15–19, 2010; Portland, Oregon
7. “Band Engineering and Magnetic Doping of Epitaxial Graphene on SiC (0001)”, APS March Meeting 2010, March 15–19, 2010; Portland, Oregon
8. “Activation of CO_2 on transition metal surfaces and oxide supported metal thin films”, 2009 APS March Meeting, March 16–20, 2009; Pittsburgh, Pennsylvania
9. “Local dielectric permittivity profiles of sapphire/polypropylene interfaces”, 2009 APS March Meeting, March 16–20, 2009; Pittsburgh, Pennsylvania
10. "Microscopic, Macroscopic, and Multi-Scale Modeling of Capacitor Dielectrics and Composites," J. Bernholc, M. Buongiorno Nardelli, L. Yu, V. Ranjan, ONR Capacitor Program Review, Hilton Head, South Carolina, March 2008.
11. "First-principles investigation of high energy density in PVDF copolymers," V. Ranjan, L. Yu, M. Buongiorno Nardelli and J. Bernholc, APS March Meeting, New Orleans, Louisiana, 2008.
12. "Equivalence of dipole correction and Coulomb cutoff techniques in supercell calculations," L. Yu, V. Ranjan, W. Lu, M. Buongiorno Nardelli and J. Bernholc, APS March Meeting, New Orleans, Louisiana, 2008.
13. “Band Engineering in C/BN Nanoribbons”, Jeff Mullen and M. Buongiorno Nardelli, APS March Meeting, New Orleans, Louisiana, 2008.
14. "Multiscale simulations of high performance capacitors and nanoelectronic devices," J. Bernholc, V. Ranjan, X. Zheng, G. Kim, W. Lu, L. Yu, and M. Buongiorno Nardelli, DoD HPC User Group Conference, Seattle, Washington, July 2008.
15. "Multiscale simulations of high performance capacitors and nanoelectronic devices," J. Bernholc, V. Ranjan, F. Ribeiro, W. Lu, L. Yu, and M. Buongiorno Nardelli, DoD HPC User Group Conference, Pittsburgh, Pennsylvania, June 2007.
16. "Microscopic, Macroscopic, and Multi-Scale Modeling of Capacitor Dielectrics and Composites," J. Bernholc, M. Buongiorno Nardelli, ONR Capacitor Program Review, Baltimore, Maryland, March 2007.
17. "Mechanisms for achieving high energy density in PVDF: a first-principles investigation," V. Ranjan, L. Yu, M. Buongiorno Nardelli, and J. Bernholc, APS March Meeting, Denver, Colorado, 2007.

18. "Electronic transport through alkane chains: the case of end group functionalization," G. Kim, W. Lu, S. Wang, M. Buongiorno Nardelli, and J. Bernholc, APS March Meeting, Denver, Colorado, 2007.
19. "Phase Transformations and High Energy Density in Ferroelectric Polymers, V. Ranjan, L. Yu, M. Buongiorno Nardelli and J. Bernholc, The Nineteenth Annual Workshop on Recent Developments in Electronic Structure Methods, Raleigh, North Carolina, June 2007.
20. Equivalence of dipole correction and Coulomb cut-off in supercell calculations, 19th Annual Workshop on Recent Developments in Electronic Structure Methods, NCSU, 13-15 June, 2007
21. Mechanisms for achieving high energy density in PVDF: a first-principles investigation, APS March Meeting, March 6, 2007 in Denver, CO
22. Maximally Localized Wannier Functions: Ultrasoft Pseudopotentials and Related Applications, CECAM-psi_k workshop "Maximally Localized Wannier Functions: Concepts, Applications, and Beyond", 27-29 June, 2007, Lyon, France.
23. Sujata Paul, Erik E. Santiso and Marco Buongiorno Nardelli, Sequestration and selective oxidation of Carbon Monoxide in graphene, 2007 AIChE Annual Meeting, Salt lake city, Utah
24. Sujata Paul, Erik E Santiso and Marco Buongiorno Nardelli, Mechanism of growth of graphitic edge in carbon monoxide atmosphere, 2007 APS March Meeting, Denver, Colorado,
25. Sujata Paul, Erik E Santiso and Marco Buongiorno Nardelli, Mechanism of growth of graphitic edge in carbon monoxide atmosphere, The 3rd Annual NC State University Graduate Student Research Symposium 2007, Raleigh, North Carolina.
26. Sujata Paul, Erik E. Santiso, M. Nunez and Marco Buongiorno Nardelli, Theoretical Design of Nanostructured Materials for CO2 Adsorption, Activation and Reduction, 2007 APS March meeting (Poster), Denver Colorado
27. Electronic transport through alkane chains: the case of end group functionalization, 2007 APS March Meeting, March 5–9, 2007; Denver, Colorado
28. E.E. Santiso, K.E. Gubbins, M. Buongiorno Nardelli, "Effect of Confinement on the Isomerization Dynamics of Small Hydrocarbons - The Shape Catalytic Effect", 9th International Conference on Fundamentals of Adsorption, Giardini Naxos, Sicily - Italy (2007)
29. E.E. Santiso, M. Buongiorno Nardelli, "A Double Exponential Effect of Confinement on Reaction Rates", Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City (2007)
30. "Methane Decomposition over Graphene Edges for CO- and CO2 – Free Hydrogen Production", L. Huang, E.E. Santiso, K.E. Gubbins and M. Buongiorno Nardelli, Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, November 4-9, 2007.
31. " First Principles Investigation of Polymer-Ceramic Interfaces and Composites", APS March Meeting, Baltimore, March 2006
32. "Carbon-based nanostructured materials for enhanced H2 production", APS March Meeting, Baltimore, March 2006
33. "First principles theory of metal-oxide interfaces: the Schottky-Mott theory revisited", APS March Meeting, Baltimore, March 2006
34. "Surface and Interface Structures of Crystalline Oxides on Silicon (COS)", APS March Meeting, Baltimore, March 2006

35. E.E. Santiso, M.K. Kostov, K.E. Gubbins, A.M. George, M. Buongiorno Nardelli, "Dissociation of Water on Defective Carbon Substrates", Annual Meeting of the American Institute of Chemical Engineers, San Francisco, CA(2006).
36. E.E. Santiso, K.E. Gubbins, A.M. George, M. Buongiorno Nardelli, "The Influence of Physical Interactions on Chemical Reactions in Confinement" (Poster), Annual Meeting of the American Institute of Chemical Engineers, San Francisco, CA (2006).
37. E.E. Santiso, A.M. George, M.K. Kostov, M. Buongiorno Nardelli, K.E. Gubbins, "Effect of Confinement on Chemical Reactions" (Poster), Winner of the Inaugural Award of the Computational Molecular Science and Engineering Forum of the American Institute of Chemical Engineers (CoMSEF), Annual Meeting of the American Institute of Chemical Engineers, San Francisco, CA(2006).
38. S. Paul, E. Santiso, M. Nuñez, M.Buongiorno Nardelli, "Theoretical Design of Nanostructured Materials for CO2 Adsorption, Activation and Reduction" (Poster), Bangalore Summer School on Electronic Structure Methods and their Applications/Conference on Computational Materials Theory, Bangalore, India (2006).
39. E.E. Santiso, M.K. Kostov, K.E. Gubbins, A.M. George, M.Buongiorno Nardelli, "Confinement Effects on Chemical Reactions – Toward an Integrated Rational Catalyst Design", 6th International Symposium on Surface Heterogeneity Effects in Adsorption and Catalysis on Solids, Zakopane, Poland (2006)
40. A. Calzolari, A. Ferretti, and M. Buongiorno Nardelli "Ab initio electronic transport in spin-polarized systems " Conference on "Computational Magnetism and Spintronics" CompMag 2006 October 2nd - 4th (2006) Forschungszentrum Jülich, Germany,
41. A. Calzolari and M. Buongiorno Nardelli, "Electronic and Transport Properties of Artificial Gold Chains on NiAl(110)", ICN+T International conference on nanoscience and nanotechnology, Jul 30 -Aug 4 (2006) Basel, Switzerland.
42. A. Calzolari, A. Ferretti, B. Bonferroni, M. Buongiorno Nardelli, E. Molinari "Electronic transport through Wannier functions: from molecular to solid state systems", CECAM workshop on: "Quantum Transport and non-adiabatic electron evolution from first principles approaches", Monday 4th to Friday 8th of December, (2006) Lyon, France
43. "Theory of CO adsorption on linear gold chains: electronic properties and transport", IUVSTA2004, Venice, June 2004.
44. "The interface phase and the Schottky barrier for a crystalline dielectric on silicon", APS March meeting, Montreal, CA, March 2004.
45. "Theory of CO adsorption on linear gold chains: electronic properties and transport", APS March meeting, Montreal, CA, March 2004.
46. "Effects of Mechanical Deformations on the Electrical Properties of Single and Multiwall Carbon Nanotubes", A. Pantano, D.M. Parks, M.C. Boyce and M. Buongiorno Nardelli, APS March meeting, Montreal, CA, March 2004.
47. "Effects of Mechanical Deformations on the Electrical Properties of Single and Multiwall Carbon Nanotubes", A. Pantano, D.M. Parks, M.C. Boyce and M. Buongiorno Nardelli, Carbon 2004, Providence, RI, July 2004.

48. "Ab initio correlated transport properties of molecular junctions", A. Ferretti, A. Calzolari, R. Di Felice, E. Molinari, F. Manghi, M. Buongiorno Nardelli and M. J. Caldas, ADMOL 2004, Dresden, February 2004.
49. “Theory of adsorption on linear gold chains: electronic properties and transport”, A. Calzolari, C. Cavazzoni and M. Buongiorno Nardelli, ADMOL 2004, Dresden, February 2004.
50. “Ab initio transport properties of carbon-based nanostructures”, A. Calzolari, N. Marzari and M. Buongiorno Nardelli, MRS fall meeting, Boston, MI, December 2003.
51. “Ab initio quantum conductance form maximally localized Wannier functions”, Y. Lee, A. Calzolari, M. Buongiorno Nardelli, N. Marzari, MRS fall meeting, Boston, MI, December 2003.
52. “Transport properties of linear atomic chains from first principles”, A. Calzolari, N. Marzari and M. Buongiorno Nardelli, HCIS30, Modena 2003.
53. “Ab initio theory of geometry, conductance and charging energy of a single-wall carbon nanowire”, K. McCall, Q. Zhao and M. Buongiorno Nardelli, II annual NCSU undergraduate summer research program symposium, Aug. 2003
54. “Transport properties of linear atomic chains from first principles”, A. Calzolari, N. Marzari and M. Buongiorno Nardelli, INFMeeting 2003, Genova, June 2003.
55. “Electronic Structure and bonding at Si/Oxide interfaces”, APS march meeting, Austin TX, March 2003.
56. “Polar properties of ferroelectric polymers from first principles”, S. Nakhmanson, M. Buongiorno Nardelli, J. Bernholc, APS march meeting, Austin TX, March 2003
57. “Ab initio quantum conductance form maximally localized Wannier functions”, Y. Lee, A. Calzolari, M. Buongiorno Nardelli, N. Marzari, APS march meeting, Austin TX, March 2003
58. “Electronic Structure and Bonding at SrO/Si(100) Interfaces”, APS March meeting, Indianapolis, Indiana, March 2002.
59. ``Bending nanotubes: device design via mechanical relaxation", APS March meeting, Atlanta, Georgia, March 1999.
60. ``Growth and mechanical properties of carbon nanotubes", MRS fall meeting, Boston, MA., Dec. 1999.
61. ``Theory of Interfaces and Surfaces in Wide-Gap Nitrides. " 24th Conference on the Physics and Chemistry of Semiconductor Interfaces, Research Triangle Park, NC, January 1997.
62. ``Theory of Interfaces in Wide-Gap Nitrides." MRS Fall Symposium, Boston, Massachusetts, 1996.
63. ``Bulk and Interfacial Properties of Nitride Semiconductors." APS March Meeting, St. Louis, Missouri, 1996.
64. ``Low energy vibrations at InSb(110) surface." 19th Annual Meeting on Advances in surfaces and interfaces physics, Modena, Italy December 1994.
65. ``Substrate-driven ordering of Sexi-Thiophene oligomers on the (1x2)Au(110) surface." 19th Annual Meeting on Advances in surfaces and interfaces physics, Modena, Italy, December 1994.
66. ``New developments in atom-surface scattering theory." University of Nottingham, Nottingham, UK, 15 November 1994.

67. ``Ab-initio lattice dynamics from density functional methods: theory and applications.", Universite' de Marne-la-Vallee, Paris, France, 30 June 1994.
68. ``Ab-initio theory of He scattering from semiconductor surfaces: InSb(110) a case study.", 13o Convegno nazionale di fisica teorica e struttura della materia, Fai della Paganella, Italy, 6-9 April 1994.
69. ``Phonon softening and low symmetry phases of Cesium Halides.", 13o Convegno nazionale di fisica teorica e struttura della materia, Fai della Paganella, Italy, 6-9 April 1994.
70. ``Introduction to Density Functional Theory electronic structure calculations and applications to semiconductor surfaces.", AREA di Ricerca di Trieste, Italy, 13 January 1993.
71. ``Phonon softening and low symmetry phases of Cesium Iodide.", AREA di Ricerca di Trieste, Italy, 20 October 1993.
72. ``Two-Grid algorithm for fast convergence in self-consistent electronic structure calculations.", round table on ``Minimization Strategies in Computer Simulations", Trieste, Italy, 16 March 1993.
73. ``Phonon softening and low symmetry phases of Cesium Iodide.", Electronic structure of solids, Cambridge, UK, 12-17 September 1992.
74. ``Phonon softening and low symmetry phases of Cesium Iodide.", Supercomputing in condensed matter physics, Ascona, Switzerland, 22-26 June 1992.
75. ``Hydrogen adsorption on Si(111) surfaces.", 12th European Conference on Surface Science, Stockholm, Sweden, 8-12 September 1991.
76. ``Vectorization of algorithms for first-principles electronic structure: diagonalization of large matrices.", International Conference on ``Supercomputing tools for science and engineering", Pisa, Italy, December 1989.