Arrigo Calzolari.

Present Position &Appointments
- Oct. 2010 – present Researcher CNR-NANO S3 Modena, IT
- Nov. 2012 – present Adjunct Professor Physics Dept., Univ. North Texas, Denton TX, USA

Education
- 02/2003 Ph.D. in Physics Univ. Modena and Reggio E.
- 07/1999 Laurea in Physics(cum laude) Univ. Modena and Reggio E.

Previous Professional Experiences
- 09/2009 – 09/2010 Researcher CNR-IOM DEMOCRITOS, Trieste, IT
- 07/2007 – 08/2009 Researcher CNR-INFM S3, Modena, IT
- 03/2003 – 06/2007 Postdoc CNR-INFM S3, Modena, IT

Research
My research activity is focused on the *ab initio* simulations – within the Density Functional Theory (DFT) framework and beyond (TDDFT) - of the structural, electronic, optical and transport properties of nanostructures, molecules, surfaces and interfaces, for solar cells, molecular electronics and nanotechnology applications. The research activity deals both with the application of state-of-the-art packages for (TD)DFT calculations to interesting physical systems, and with the development and the implementation of original methods for the evaluation of the electronic and thermal transport properties in nanostructures.
Specific themes of research:
- (Bio)molecules and low-dimensional systems: molecular dyes (**anthocyanins** [see e.g. Refs. 10, 19, 23], catecholates, Ru-based), organometallic complexes (porphyrins, phthalocyanins), nucleic acids, polypeptides, organic (PPV) and inorganic (MMX, Co-bioxolane) polymers, wires, CNT and graphene.
- Thermodynamic stability, dynamical evolution and **optical properties of molecules and nanostructures in solution at finite temperature** [see e.g. Refs. 10, 11, 18, 19, 23].
- Hybrid organic/inorganic interfaces including semiconductor (Si, SiC, III-V, II-VI), metal-oxide (ZnO) and metal (Au, Cu, Ag, NiAl) substrates, for photovoltaic and electronic devices.
- Electronic and heat transport in nanostructures and Wannier Functions: method development and code implementation (WanT PROJECT, www.wannier-transport.org) as well as applications to systems scientifically relevant for nanotechnology applications.

Scientific activity
- Author of more than 50 original articles in journals and 6 scientific review articles and book chapters abstracted by ISI, including Nature Materials, Nature Nanotechnology, Physical Review Letters, Journal of American Chemical Society, Applied Physics Letters, J. of Physical Chemistry Letters. H-index 19, (source: ISI Web of Science Jan 2013). [see full list of publications].
- 7 invited talks to peer-reviewed internationally established conferences, 5 invited presentations/lectures to international workshops and advanced schools (since 2008), and 4 invited seminars in international scientific institutions.
- Program Committee of National Workshop on "Surfaces, Interfaces and Functionalization Processes in Organic compounds and Applications", SINFO, June 20 – 22, 2012, Parma Italy.
- Referee for condensed-matter and chemical-physics journals, including Phys. Rev. Lett., J. Am. Chem. Soc., J.Phys. Chem, J. Phys.: Cond. Matt., Nanotech., Europhys. Lett., Chem. Phys. Lett.
- Co-Supervision and training of graduate and undergraduate students
- Lecturer at University of Modena e Reggio E.: exercise on mechanics and electromagnetism (2003-2008) and quantum mechanics (2002).

Collaborations & Partnerships
- Prof. Marco Buongiorno Nardelli, Department of Physics, University of North Texas, Denton TX, USA. The collaboration is active since 2002. The joint activity of the two partners led development of a novel numerical methodology for the evaluation of electronic and heat transport in nanostructures and the publication of many scientific papers.
- Prof. Stefano Baroni, SISSA, Trieste, IT. The collaboration is active since 2009 and deals with the optical

properties and color simulation of molecular dye in solution, via TDDFT approaches.
- Further national and international scientific collaborations include: F. Zamora and J. Gomez-Herrero (Univ. Autonoma, Madrid ES), M.J. Caldas and H. Petrilli (Univ. de Sao Paulo, Brazil), D.B. Dougherty and D. Shultz (North Carolina State University, Raleigh, NC USA), T. Jayasekera (Southern Illinois University, Carbondale, IL USA), M.G. Betti and C. Mariani (Univ. La Sapienza, Rome IT), T. Virgili (Politecnico Milano, IT), M. Pedio and S. Fabris (CNR-IOM, Trieste, IT).

Projects
- Participation to scientific projects funded by regional (Laboratorio Regionale Emilia Romagna NANOFABER 2005-2007), national (PRIN-2008, PRIN-2006, PRIN-2004, FIRB-NOMADE 2003-2006) and international (EC NEST STREP "Prosurf" 2006-2009; EC IST FET-Open "DNA-BASED NANODEVICES" 2006-2009; EC IST FET-Open "DNA-BASED NANOWIRES" 2003-2005) agencies.
- Participation/coordination to/of supercomputing projects, including PRACE 2012 (EU project), ISCRA 2010-2011, DEISA 2008 (EU project), CNMS-Oak Ridge 2011, CINECA 2001-2009.

List of Publications

1. **A. Calzolari**, T. Jayasekera, K.W. Kim, and M. Buongiorno Nardelli, "Ab initio thermal transport properties of nanostructures from density functional perturbation theory", J. Phys.: Cond. Matter. **24**, 492204 (2012).
2. **A. Calzolari**, Y. Chen, G.F. Lewis, D. B. Dougherty, D. Shultz, and M. Buongiorno Nardelli, "Complex Materials for Molecular Spintronics Applications: Cobalt bis(dioxolene) Valence Tautomers, from Molecules to Polymers", J. Phys. Chem. B **161**, 13141 (2012).
3. **A. Calzolari**, M. Bazzani and A. Catellani, "Dipolar and charge transfer effects on the atomic stabilization of ZnO polar surfaces", Surf. Sci. **607**, 181 (2013).
4. G. Givaja, O. Castillo, E. Mateo, A. Gallego, C.J. Gómez-García, **A. Calzolari**, R. di Felice, and F. Zamora "Electrical Behaviour of Heterobimetallic MM´X-Chain Polymers PtM(EtCS2)4I (M = Ni, Pd)", Chem. Eur. J. **18**, 15476 (2012).
5. R. Mao, B. D. Kong, K. W. Kim, T. Jayasekera, **A. Calzolari**, and M. Buongiorno Nardelli, "Phonon Engineering in Nanostructures: Controlling Interfacial Thermal Resistance in Graphene/Dielectric Systems", Appl. Phys. Lett. **101**, 113111 (2012).
6. **A. Calzolari**, A. Ruini, and A. Catellani, "Surface effects on catecholic chemistry at hexagonal substrates: structural and electronic properties", J. Phys. Chem. C **116**, 17158 (2012).
7. M. G. Betti, P. Gargiani, C. Mariani, S. Turchini, N. Zema, S. Fortuna, **A. Calzolari**, and S. Fabris, "Formation of hybrid electronic states in FePc chains mediated by the Au(110) surface", J Phys. Chem. C **116**, 8657 (2012).
8. S. Fortuna, P. Gargiani, M.G. Betti, C. Mariani, **A. Calzolari**, S. Modesti and S. Fabris, "Molecule-driven substrate reconstruction in the two-dimensional self-organization of Fe-phthalocyanines on Au(110)", J. Phys. Chem. C **116**, 6251 (2012).
9. A. Catellani and **A. Calzolari**, "Functionalization of SiC(110) surfaces via porphyrin adsorption: ab initio results", J. Phys. Chem. C **116**, 886 (2012).
10. O.B. Malcioglu, **A. Calzolari**, R. Gebauer, D. Varsano and S. Baroni, "Dielectric and thermal effects on the optical properties of natural dyes: a case study on solvated cyanin", J. Am. Chem. Soc. **133**, 15425 (2011).
11. G. Cicero, **A. Calzolari**, S. Corni, and A. Catellani, "Thermally induced anomalous wetting layer at the Au(111) surface", J. Phys. Chem. Lett. **2**, 2582 (2011).
12. **A. Calzolari**, A. Ruini, and A. Catellani, "Anchor group versus conjugation: towards the gap-state engineering of functionalized ZnO(10-10) surface for optoelectronic applications", J. Am. Chem. Soc. **133**, 5893 (2011).
13. M. Bazzani, A. Neroni, **A. Calzolari**, and A. Catellani, "Optoelectronic properties of Al:ZnO: Critical dosage for an optimal transparent conductive oxide", Appl. Phys. Lett. **98**, 121907 (2011).
14. M. Fanetti, **A. Calzolari**, P. Vilmercati, C. Castellarin-Cudia, P. Borghetti, G. Di Santo, L. Floreano, A. Verdini, A. Cossaro, I. Vobornik, E. Annese, F. Bondino, S. Fabris and A. Goldoni, "The structure and the molecule-substrate interaction in a Co-octaethylPorphyrin monolayer on the Ag(110) surface", J. Phys. Chem. C **115**, 11560 (2011).
15. **A. Calzolari**, A. Ruini, C. Cavazzoni, and M. J. Caldas, "Substitutional impurities in PPV crystals: an intrinsic donor-acceptor system for high Voc photovoltaic devices", J. Phys. Chem C **114**, 19535 (2010).
16. Y. Chen, T. Jayasekera, **A. Calzolari**, K.W. Kim, and M. Buongiorno Nardelli, "Thermoelectric properties of graphenenanoribbons, junctions and superlattices", J. Phys.: Condens. Matter **22**, 372202 (2010).
17. C. Cocchi, D. Prezzi, **A. Calzolari**, and E. Molinari, "Spin-transport selectivity upon Co adsorption on antiferromagnetic graphenenanoribbons", J. Chem. Phys., **133**, 124703 (2010).
18. **A. Calzolari**, G. Cicero, C. Cavazzoni, R. Di Felice, A. Catellani and S. Corni, "Hydroxyl-rich beta-sheet adhesion to the gold surface in water by first-principle simulations", J. Am. Chem. Soc. **132**, 4790 (2010).
19. **A. Calzolari**, S. Monti, A. Ruini, and A. Catellani, "Hydration of cyanin dyes", J. Chem. Phys. **132**, 114304 (2010); also selected for the March 2010 issue of JCP: BioChemical Physics.
20. A. Guijarro, O. Castillo, L. Welte, **A. Calzolari**, P. J. Sanz Miguel, C. J. Gómez-García, D. Olea, R. Di Felice, J. Gómez-Herrero, and F. Zamora, "MMX as conductors from single crystals to nanostructures", Adv. Funct. Mater. **20**, 1451 (2010).

21. L. Welte, **A. Calzolari**, R. Di Felice, F. Zamora, and J Gómez-Herrero, "Highly conductive nanoribbons of coordination polymers", Nat. Nanotech. **5**, 110 (2010).
22. **A. Calzolari**, W. Jin, J. Reutt-Robey, M. Buongiorno Nardelli, "Substrate-Mediated Intermolecular Hybridization in Binary Phthalocyanine Superstructures", J. Phys. Chem. C **114**, 1041 (2010).
23. **A. Calzolari**, D. Varsano, A. Ruini, A. Catellani, R. Tel-Vered, H.B. Yildiz, O. Ovits, I. Willner, "Optoelectronic properties of natural cyanin dyes", J. Phys. Chem. A **113**, 8801 (2009).
24. **A. Calzolari** and A. Catellani, "Water adsorption on non-polar ZnO(10-10) surface: a microscopic understanding", J. Phys. Chem C **113**, 2896 (2009).
25. D.A. Ryndyk, E. Shapir, D. Porath, **A. Calzolari**, R. Di Felice, and G. Cuniberti, "Scanning Tunneling Spectroscopy of Single DNA Molecules", ACSnano**3**, 1651 (2009).
26. A. Guijarro, Os. Castillo, **A. Calzolari**, P. J. Sanz Miguel, C. J. Gómez-García, R. di Felice, and F. Zamora, "Electrical conductivity in Platinum-dimer columns", Inorg. Chem. **47**, 9736 (2008).
27. L. Zoppi, **A. Calzolari**, A. Ruini, A. Ferretti, and M.J. Caldas "Defect-induced effects on carrier migration through one-dimensional poly-para-phenilenevinylene chains", Phys. Rev. B **78**, 165204 (2008).
28. B. Bonferroni, A. Ferretti, **A. Calzolari**, A. Ruini, M.J. Caldas, and E. Molinari, "Oxygen-mediated electron transport through hybrid silicon-organic interfaces", Nanotechnology **19**, 285201 (2008).
29. **A. Calzolari**, R. Di Felice, S.S. Alexander, and F. Zamora, "Metallicity in individual MMX chains", J. Am. Chem. Soc. **130**, 5552 (2008).
30. E. Shapir, H. Cohen, **A. Calzolari**, C. Cavazzoni, D. A. Ryndyk, G. Cuniberti, A. Kotlyar, R. Di Felice and D. Porath, "Electronic structure of single DNA molecules resolved by transverse scanning tunneling spectroscopy", Nat. Mater. **7**, 68 (2008).
31. C. Baldacchini, C. Mariani, M.G. Betti, I. Vobornik, J. Fujii, E. Annese, G. Rossi, A. Ferretti, **A. Calzolari**, R. Di Felice, A. Ruini, and E. Molinari, "Symmetry lowering of pentacene molecular states interacting with a Cu Surface", Phys. Rev. B **76**, 245430 (2007).
32. 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).
33. G. P. Brandino, G. Cicero, B. Bonferroni, A. Ferretti, **A. Calzolari**, C. M. Bertoni, and A. Catellani, "Polarization properties of 1-100 and 11-20 SiC surfaces from first principles", Phys. Rev. B **76**, 085322 (2007).
34. **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).
35. A. Ferretti, C. Baldacchini, **A. Calzolari**, R. Di Felice, A. Ruini, E. Molinari, and M. G. Betti, "Mixing of electronic states in pentacene adsorption on copper", Phys. Rev. Lett. **99**, 046802 (2007).
36. A.A. Stekolnikov, K. Seino, F. Bechstedt, S. Wippermann, 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).
37. M.J. Caldas, **A. Calzolari**, and C.S. Cucinotta, "Trimming Si Surface for molecular electronics", J. Appl. Phys. **101**, 081719 (2007).
38. A. Ferretti, **A. Calzolari**, B. Bonferroni, R. Di Felice, "Maximally localized Wannier functions from PAW or ultrasoftpseudopotentials", J. Phys.: Condens. Matter **19**, 036215 (2007).
39. M. Cavallari, **A. Calzolari**, A. Garbesi, and R. Di Felice, "Stability and Migration of Metal Ions in G4-wires by Molecular Dynamics Simulations", J. Phys. Chem B **110**, 26337 (2006).
40. **A. Calzolari**, A. Ruini, M.J. Caldas, and E. Molinari, "Surface nano-patterning through styrene adsorption on Si(100)", Phys. Rev. B **73**, 125420 (2006) .
41. R. Di Felice, **A. Calzolari**, Anna Garbesi, S. S. Alexandre, and J. M. Soler, "Strain-dependence of the electronic properties in periodic quadruple helical G4-wires", J. Phys. Chem. B **109**, 22301(2005).
42. A. Ferretti, **A. Calzolari**, R. Di Felice, F. Manghi, "First principles theoretical description of transport including electron-electron correlation, Phys. Rev. B **72**, 125114 (2005).
43. **A. Calzolari** and M. Buongiorno Nardelli, "First principle theory of artificial metal chains on NiAl(110) surface", Phys. Rev. B **72**, 045416 (2005).
44. H. Zhang, **A. Calzolari**, and R. Di Felice, "Ferromagnetic alignment of metal ions in a DNA-mimic double helix", J. Phys. Chem. B **119**, 15345 (2005).

45. A. Ferretti, **A. Calzolari**, R. Di Felice, F. Manghi, M.J. Caldas, M. Buongiorno Nardelli, and E. Molinari, "First principle theory of correlated transport through nano-junctions", Phys. Rev. Lett. **94**, 116802 (2005).
46. **A. Calzolari**, C. Cavazzoni, and M. Buongiorno Nardelli, "Electronic and transport properties of artificial gold chains", Phys. Rev. Lett. **93**, 096404 (2004).
47. R. Di Felice, **A. Calzolari**, H. Zhang, "Towards metalated DNA-based structures", Nanotechnology **15**, 1256 (2004).
48. **A. Calzolari**, R. Di Felice, E. Molinari, and A. Garbesi, "Electron channels in biomolecular nanowires", J. Phys. Chem. B **108**, 2509 (2004).
49. **A. Calzolari**, N. Marzari, I. Souza and M. Buongiorno Nardelli, "Ab-initio transport properties of nanostructures from maximally-localized Wannier functions", Phys. Rev. B **69**, 035108 (2004).
50. S. Nakhmanson, **A. Calzolari**, V. Meunier, J. Bernholc, and M. Buongiorno Nardelli, "Spontaneous polarization and piezoelectricity in boron nitride nanotubes", Phys. Rev. B **67**, 235406 (2003).
51. **A. Calzolari**, R. Di Felice, E. Molinari, and A. Garbesi, "G-Quartet Biomolecular Nanowires", Appl. Phys. Lett. **80**, 3331 (2002).
52. **A. Calzolari**, R. Di Felice, E. Molinari, and A. Garbesi, "Self-assembled guanine ribbon as wide-bandgap semiconductors", Physica E **13/2-4**, 1236 (2002).
53. R. Di Felice, **A. Calzolari**, E. Molinari, and A. Garbesi, "Ab-initio study of model guanosine assemblies: The role of pi-pi coupling and band transport", Phys. Rev. B **65**, 045104-1 (2002).
54. **A. Calzolari**, C.A. Pignedoli, R. Di Felice, C.M. Bertoni, and A. Catellani, "Theory of Cs adsorption on InAs(110)", Surf. Sci. **491/1-2**, 265 (2001).
55. **A. Calzolari**, C. A. Pignedoli, R. Di Felice, C. M. Bertoni, and A. Catellani, "First-principle investigation of the formation of Cs-dimer-chains upon adsorption on InAs(110)", Surf. Sci. **454-456**, 207 (2000).

Review Articles and Book Chapters

1. L. Bellucci, G. Brancolini, **A. Calzolari**, O. Carrillo Parramon, S. Corni, and R. Di Felice, "Proteins and peptides at gold surfaces: insights from atomistic simulations", in "Proteins at Interfaces III", Edited by Horbett, T., et al. , ACS Symposium Series, American Chemical Society: Washington, DC, 2012, cap. 10, pp. 229-250.
2. **A. Calzolari** and R. Di Felice, "Surface functionalization through adsorption of organic molecules", J. Phys.: Cond Matt. **19**, 305018 (2007).
3. R. Di Felice and **A. Calzolari**, Electronic structure of DNA derivatives and mimics by Density Functional Theory, in "'Modern methods for theoretical physical chemistry of biopolymers", pp. 485-507, ed. by Evgeni B. Starikov, James P. Lewis and Shigenori Tanaka, Elsevier (2006).
4. R. Di Felice, A. Rubio, D. Varsano, and **A. Calzolari**, Electronic structure calculation for nanomolecular systems, invited paper to be published in "Introducing Molecular Electronics" edited by G. Cuniberti, K. Richter G. Fargas , Lect. Notes Phys. 680, 77 (2005). (Springer).
5. **A. Calzolari**, R. Di Felice, and E. Molinari, Electronic properties of guanine-based nanowires, Sol. St. Commun. **113**, 577 (2004) - Special Issue on "New advances on collective phenomena in one-dimensional systems", Ed. by H. Grabert and V. Pellegrini.
6. R. Rinaldi, E. Branca, R. Cingolani, R. Di Felice, **A. Calzolari**, E. Molinari, S. Masiero, G.P. Spada, G. Gottarelli, and A. Garbesi, Biomolecular electronic device based on Self-organized Deoxyguanosine nanocrystals, pp 184-192, in "Molecular Electronics II", edited by A. Aviram, M. Ratner, V. Mujica, Annals of the New York Academy of Science (Vol. 60), April 2002.

Modena 04/12/2012

Arrigo Calzolari