

ARRIGO CALZOLARI – CV

Present position and appointments

- Researcher (10/2010 - present) – Permanent staff - CNR-NANO S3 Modena, IT (www.nano.cnr.it)
- Since Nov. 2102 Adjunct Professor Physics Dept., University of North Texas, Denton TX, USA

Professional Experiences

- Collaborator (05/2013 – 05/2014) – Collaborator @ SISSA, Trieste, IT
- Researcher (09/2009 - 09/2010) CRN-IOM DEMOCRITOS, Trieste, IT (www.democritos.it)
- Researcher (07/2007 - 08/2009) CNR-INFM S3, Modena, IT
- Postdoc (03/2003 - 06/2007) CNR-INFM S3, Modena, IT

Research

My research activity is focused on the *ab initio* study - within the Density Functional Theory (DFT) framework and beyond (TDDFT) - of the structural, electronic, optical, vibrational 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 transport properties in nanostructures.

The field of research interests includes:

- Thermodynamic stability and dynamical evolution of molecules and nanostructures in water solution.
- Optical properties and color simulation of molecular dyes (e.g anthocyanins and merocyanine) in solution (see below, Refs 1-3 in the short publication list).
- Hybrid organic/inorganic interfaces
- Polymers, (bio)molecules and low-dimensional systems
- Electronic and heat transport in nanostructures and Wannier Functions - (Want PROJECT www.wannier-transport.org)

Education

- Ph.D. in Physics (01/2003)
University of Modena and Reggio E.
Supervisor: Prof. E. Molinari
Thesis: *Nucleosides-based solids as wide bandgap semiconductors: electronic properties and transport*
- Laurea (cum laude) in Physics (07/1999)
University of Modena and Reggio E.
Supervisor: Prof. C.M. Bertoni
Thesis: *Electronic Structure and Atomic Geometry in Cs Adsorption on InAs(110)*

Scientific activity

- Author of about 70 scientific papers published in international journals, and of 6 scientific review articles and book chapters. H-index=24 (source: Google scholar, May. 2014).
- Author of 8 invited talks to peer-reviewed international conferences and of 6 presentations/lectures to international workshops and advanced schools (since 2008).
- MIUR teaching qualification for professorship in Physics (theoretical condensed matter) and Physical Chemistry (2013).
- Co-supervisor of graduate and undergraduate students.
- 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

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international (EC NEST STREP "Prosur" 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 CINECA 2001-2009, DEISA (2008, 2012) e IS CRA 2010, OAK RIDGE LAB 2011, PRACE (2011, 2012, 2013)).
- Referee for scientific journals, including Phys. Rev. Lett., J. Am. Chem. Soc., J. Phys. Chem, J. Phys.. Cond. Matt., Nanotech., Europhys. Lett., Chem. Phys. Lett.
- Lecturer at national and international schools and workshop on computational materials science (4 contributions since 2008).

Lecturer at University of Modena e Reggio E., exercise on mechanics and electromagnetism (2003-2008) and quantum mechanics (2002).

Collaborations&Partnerships

National and international scientific collaborations include S. Baroni (SISSA, Trieste, IT), M.B. Nardelli (Univ. North. Texas, TX, USA), MG Betti and C. Mariani (Univ. La Sapienza, Rome IT), F. Zamora and J. Gomez-Herrero (Univ. Autonoma, Madrid ES), D. Porath and I. Willner (Hebrew Univ., Jerusalem, Israel), M.J. Caldas (Univ. de Sao Paulo, Brazil), T. Virgili (Politecnico Milano, IT), M. Pedio and S. Fabris (CNR-IOM, Trieste, IT).

Selected Publications

- O.B. Malcioglu, A. Calzolari, R. Gebauer, D. Varsano and S. Baroni, J. Am. Chem. Soc., 133, 15425 (2011).
- A. Calzolari, S. Monti, A. Ruini, and A. Catellani, J. Chem. Phys. 132, 114304 (2010).
- A. Calzolari, D. Varsano, A. Ruini, A. Catellani, R. Tel-Vered, H.B. Yildiz, O. Ovits, I. Willner, J. Phys. Chem. A 113, 8801 (2009).
- A. Calzolari, G. Cicero, C. Cavazzoni, R. Di Felice, A. Catellani and S. Corni, J. Am. Chem. Soc. 132, 4790 (2010).
- A. Calzolari and M. B. Nardelli, Sci. Rep. 3 2999 (2013).
- Pronschinske, Y. Chen, G. F. Lewis, D. A. Shultz, A. Calzolari, M. B. Nardelli, and D. B. Dougherty, Nano Letters 13 1429 (2013).
- A. Calzolari, A. Ruini, and A. Catellani, J. Am. Chem. Soc. 133, 5893 (2011).
- L. Welte, A. Calzolari, R. Di Felice, F. Zamora, and J. Gómez-Herrero, Nat. Nanotech. 5, 110 (2010).
- E. Shafir, H. Cohen, A. Calzolari, C. Cavazzoni, D. A. Ryndyk, G. Cuniberti, A. Kotlyar, R. Di Felice and D. Porath, Nat. Mater 7, 68 (2008).
- A. Calzolari, N. Marzari, I. Souza and M. B. Nardelli, Phys. Rev. B 69, 035108 (2004).

For the complete list of publications see http://amuse.nano.cnr.it/?page_id=66

Contact Details

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