CV of STEFANO FABRIS

Personal data

Name: Stefano Fabris

Education

5/7/2000	Award of the Ph.D. degree in theoretical physics, Queen's University of Belfast, United Kingdom.
1997-1999	Postgraduate Ph.D. student at the Atomistic Simulation Group, Queen's University of Belfast, United Kingdom;
24/2/1998	Award of the degree in Materials Engineering (mark: 110/110 cum laude) at the University of Trieste, Italy.
1992-1997	Regular undergraduate curriculum (five years) at the University of Trieste, Italy: Department of Materials, Faculty of Engineering.

Professional experience

2008-present	Full-time researcher at the "Istituto Officina dei Materiali" of the National Research Council (CNR) in Trieste, Italy;
2005-present	Coordinator of the theory group at the ELETTRA synchrotron facility (*Sincrotrone Trieste)*, Trieste, Italy;
2005	Visiting scientist at the Max-Planck-Institut für Festkörperforschung, Stuttugart.
2004-2008	Tenure-track researcher at the INFM-CNR DEMOCRITOS Simulation Center (Tenured in 2008);
2003-2004	Postdoctoral research fellow at the INFM-CNR DEMOCRITOS (Promoted to tenure track in 2004);
2000	Visiting scientist at the Atomistic Simulation Group of the Queen's University of Belfast.
2000-2002	Postdoctoral research fellow at the Max-Planck-Institut für Metallforschung, Stuttgart, Germany.

Scientific publications and presentations at conferences

Since year 2000, I have published 30 papers in international refereed journal, some of them with high impact factor, including Science, Angewandte Chemie International Edition, Journal of the American Chemical Society, Physical Review Letters, and Nano Letters. According to the ISI web of knowledge, these scientific contributions have been cited more than 970 times (350 times since January 2010). My h-index is 15. I have organized 7 international conferences/workshops/schools.

The interest into my scientific achievements is corroborated by 20 invitations at international conferences, including the European Conference on Surface Science (ECOSS-2006), the American Chemical Society fall meeting (2007), and the European Physical Society meeting (EPS-CMD 22, 2008). I teach at the Faculty of Engineering of the University of Trieste the course "Modellizzazione su base nano e microstrutturale", and have been invited as a lecturer to present several thematic lectures at international schools/workshops and research institutes.

Teaching experiences

- "Modellizzazione su base nano e microstrutturale" – Faculty of Engineering – Department of materials - 40 hours.
- Supervisor of 4 postdoctoral fellows (S. Fortuna, T. Sun, M. Huang, H. Üstünel, M. Farnesi) of the CNR DEMOCRITOS National Simulation Center; 2 Ph.D students (A. Mosca Conte, C. Ma) and 1 Master student (G. Fratesi) of the International School for Advanced Studies SISSA (www.sissa.it); 1 Master student (L. Szabova) of the Charles University in Prague (Check Republic); and co-supervisor of 1 Ph. D. student (X. Wang) of the Tianjing University (China).
- Lecturer at national and international workshops and schools on fundamentals and applications of density functional theory calculations to materials science (8 contributions since 2004).
- Teaching assistant in the Master of Science (MSc) courses "*Electronic structure of condensed matter*" I and II (2000-2001), University of Stuttgart (Dr. Ch. Elsässer).
- Teaching assistant in the MSc courses (1997-1999), Physics Department, Queen's University of Belfast (Dr. A. T. Paxton).

Organisation of national and international conferences

- *Workshop on New Materials for Renewable Energy*, October 2011, SISSA and International Center of Theoretical Physics, Trieste.
- *14th International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods*, Jan 2011, International Center of Theoretical Physics (ICTP), Trieste. (about 20 invited speakers and 250 planned participants);
- *10th ECSAC conference on "Sustainable Energy: Challenges and Opportunities"*- August 2010, Losinj (Croatia).
- Psi-K symposium *Catalysis from first principles - Energy conversion and storage,* 12-16 Sept. 2010, Berlin (Germany). Web site: www.fhi-berlin.mpg.de/th/Meetings/psik_2010/ (about 7 invited speakers in the symposium);
- *Computer Simulation of Surface and Interface -Phenomena*, ELETTRA synchrotron laboratory, 15-16 Dec. 2005, Trieste (Italy). Web site: www.elettra.trieste.it/um13/w2-index.html (15 invited speakers, about 100 participants)
- *Ab-initio simulation of the electronic, structural and dynamical properties of materials*, 26-30 Sept. 2005, SLACS center of the CNR, Cagliari (Italy). Web site: www.democritos.it/events/espresso-tutorial-2.php;
- *Numerical methods for calculating the electronic, structural, and dynamical properties of materials.* March 2004. CINECA supercomputing center, Bologna.

Funding

- Italian research council and National Institute for the Physics of Matter (CNR-INFM): 3 projects between 2005 and 2009. 110000 €
- EU – Marie Curie International Re-integration Grant: host of 1 project started in May2009, *Water splitting Catalysts for Artificial Photosynthesis.* 100000 €
- Regional grant from *Friuli Venezia Giulia: Nanocatalysis on carbon-based materials. 2008-2010* - 280000 €
- PRIN - MINISTERO DELL'ISTRUZIONE DELL'UNIVERSITÀ E DELLA RICERCA: *Computational microscopy and spectroscopy of metal-supported organometallic nanostructures, 2010; 40000* €
- Sincrotrone Trieste s.r.l (ELETTRA): *Theory@Elettra group, 2006-2011, 300000* €

Invited presentations at conferences and schools

- 2010: *Energy Materials Workshop,* 7-9 September 2010, Thomas Young Center, London, UK.

- 2010: CECAM workshop *"Electronic-structure challenges in materials modeling for energy applications"*, 1-4 June 2010, Lausanne, CH.
- 2010: *Workshop on Cerium Oxide*, 23-25 June 2010, CNR-NANO Modena, Italy.
- 2009: *Advanced School and International Conference on DFT and its Applications in Nanosciences*, 19-29 October 2009, Marmaris, Turkey.
- 2009: *Discovery in Basic Energy Sciences: The Role of Computing at the Extreme Scale*, 13-15 Aug. 2009, Washington, USA.
- 2009: *Latin American School On Computational Materials Science*, 19-30 Jan. 2009, Santiago, Chile.
- 2008: 22nd General Conference of the Condensed Matter Division of the European Physical Society Meeting, Rome, Italy.
- 2008: Winter School on *Applications of Computer Simulation and Modelling in Contemporary Solid State Physics and Nanotechnology*, Marmaris, Turkey.
- 2007: International Workshop on *Materials Science and Nano-Engineering*, Awaji, Japan.
- 2007: American Chemical Society meeting, Boston
- 2006: European Conference on Surface Science (ECOSS 24), Paris
- 2006: Workshop on *Nanostructured oxide surfaces*, Torino.
- 2006: Set of lectures at the CECAM tutorial *Simulating matter at the nano-scale using density-functional theory, pseudopotentials and plane waves,* Lyon, France.
- 2006: EUROCORES workshop *"Functional molecular nanostructures"*, Kloster Irsee, Germany.
- 2005: International Workshop on *Computer simulation of surface and interface phenomena*, Trieste, Italy.
- 2005: International meeting *Matter, Materials, and Devices*, Genova
- 2004: Set of lectures in the *Nanoscience and Nanotechnologies School*, Losinj (Croatia)
- 2004: Psi-k international workshop *Progress in Ab Initio Computational Methods for Condensed Matter*, Paris
- 2003: Set of lectures, *International course on pseudopotential plane-wave electronic structure calculations*, International Center for Theoretical Physics, Trieste.
- 2002: International Symposium *Science and Technology of Alumina*, Schloss Ringberg of the Max Planck Institut.

Scientific responsibilities

- Coordinator of the theory group of the ELETTRA synchrotron laboratory (www.democritos.it/the-group);
- Referee for Science, Physical Review Letters, J. Am. Chem. Soc., Physical Review B, Applied Physics Letters, Advanced Functional Materials, Journal of Physical Chemistry, Journal of Chemical Physics, Surface Science, Acta Materialia, and Solid State Communications;
- Referee for the funding agency *Air Force Office of Scientific Research*;
- Referee for the Swiss Center for Scientific Computing of the ETH Zurich;
- Member of the Scientific Advisory Board of the European Network *Psi-k Ab-initio calculation of complex processes in materials* (www.psi-k.org/);
- Member of the national scientific board evaluating research grants on high-performance computing at the CINECA supercomputing center (http://infm.cineca.it/risorse/gruppo2008.html);

Publication List

1. S. Fabris, A.T. Paxton and M.W. Finnis, *"Relative energetics and structural properties of zirconia using a self-consistent tight-binding model"*, Phys. Rev. B **61**, 6617 (2000).
2. S. Fabris, A.T. Paxton and M.W. Finnis, *"Free energy and molecular dynamics calculations for the cubic-tetragonal phase transition in zirconia"*, Phys. Rev. B. **63**, 94101 (2001).
3. S. Fabris and Ch. Elsässer, *"The Sigma 13 (10-14) twin in alpha-Al2O3: A model for a general grain boundary"*, Phys. Rev. B **64**, 245117 (2001).
4. S. Fabris, A.T. Paxton and M.W. Finnis, *"A stabilization mechanism of zirconia based on oxygen vacancies only"*, Acta. Mater. **50**, 5171-5178 (2002).
5. S. Fabris, S. Nufer, Ch. Elsässer, and Th. Gemming, *"The prismatic Sigma 3 (10-10) twin boundary in alpha-Al2O3 investigated by density functional theory and transmission electron microscopy"*, Phys. Rev. B **66**, 155415 (2002).
6. S. Fabris and Ch. Elsässer, *"First-principles analysis of intergranular cation segregation to alpha-alumina twin boundaries"*, Acta Mater. **51**, 71-86 (2003).
7. S. Fabris and C. Elsässer, "Ab-initio theory of grain-boundary segregation in alumina: atomistics, energetics and electronic structure", *MRS Proceedings* **751**, (2003).
8. F. Esch, S. Fabris, L. Zhou, T. Montini, C. Africh, P. Fornasiero, G. Comelli, and R. Rosei, *"Electron localization determines defect formation on ceria substrates"*, Science **309**, 752 (2005).
9. S. Fabris, S. de Gironcoli, S. Baroni, G. Vicario, and G. Balducci, *"Taming multiple valency with density functionals: a case study of defective ceria"*, Phys. Rev. B **71**, 041102 (2005).
10. S. Fabris, G. Vicario, G. Balducci, S. de Gironcoli, and S. Baroni, *"Electronic and atomistic structures of clean and reduced ceria surfaces"*, J. Phys. Chem B **109**, 22860 (2005).
11. S. Fabris, S. de Gironcoli, S. Baroni, G. Vicario, and G. Balducci, Phys. Rev. B **72**, 237102 (2005).
12. T. Classen, G. Fratesi, G. Costantini, S. Fabris, F. L. Stadler, C. Kim, S. de Gironcoli, S. Baroni, and K. Kern, *"Templated growth of metal-organic coordination chains at surfaces"*, Angew. Chem. Int. Ed. **44**, 6142 (2005).
13. S. Clair, S. Pons, S. Fabris, S. Baroni, H. Brune, K. Kern, and J. V. Barth, *"Monitoring two-dimensional coordination reactions: directed assembly of Co-terephthalate nanosystems on Au(111)"*, J Phys. Chem B **110**, 5627 (2006).
14. G. Vicario, G. Balducci, S. Fabris, S. de Gironcoli, and S. Baroni, *"Interaction of Hydrogen with Cerium Oxide Surfaces: a Quantum Mechanical Computational Study"*, J. Phys. Chem. B **110**, 19380 (2006).
15. M. Huang and S. Fabris, *"Role of surface peroxo and superoxo species in the low-temperature oxygen buffering of ceria: Density functional theory calculations"*, Phys. Rev. B **75**, 081404, (2007)
16. A. Barinov A, H. Ustunel, S. Fabris L. Gregoratti, L. Aballe, P. Dudin, S. Baroni, and M. Kiskinova, "*Defect-controlled transport properties of metallic atoms along carbon nanotube surfaces*", Phys. Rev. Lett. 99, 046803 (2007).
17. T. Classen, G. Fratesi, G. Costantini, S. Fabris, F. L. Stadler, C. Kim, S. de Gironcoli, S. Baroni, and K. Kern, *Angew. Chem.* **117**, 6298 (2005).
18. I. Vobornik, J. Fujii, G. Panaccione, S. Fabris, S. Baroni, and G. Rossi, "*Three-dimensional tomography of the beryllium fermi surface: Surface charge redistribution*", Phys. Rev. Lett. 99, 166403 (2007).

19. T. Classen, M. Lingenfelder, Y. Wang, R. Chopra, G. Costantini, K. Kern, G. Fratesi, S. Fabris, S. Baroni, S. Haq, R. Raval, *"Hydrogen and coordination bonding supramolecular structures of trimesic acid on Cu(110)"*, J. Phys. Chem. A **111**, 12589 (2007).
20. M. Hinterstein, X. Torrelles, R. Felici, J. Rius, M. Huang, S. Fabris, H. Fuess and M. Pedio *Looking underneath the fullerenes on Au(110): formation and ordering of surface substrate vacancies* Phys. Rev. B 77, 153412 (2008)
21. M. Huang and S. Fabris, *"CO adsorption and oxidation on ceria surfaces from DFT+U calculations"*, J. Phys. Chem. C **112**, 8643 (2008).
22. L. Vitali, S. Fabris, A. Mosca Conte, S. Brink, M. Ruben, S. Baroni and K. Kern, *"Two-dimensional arrays of Bis(phthalocyaninato)terbium(III) single molecular magnets on Cu (111)"*, Nano Letters **8**, 3364 (2008).
23. A. Mosca Conte, S. Fabris, and S. Baroni *Properties of Pt-supported Co nanomagnets from relativistic density functional theory calculations* Phys. Rev. B 78, 014416 (2008)
24. A. Barinov,, O. B., Malcioglu, S. Fabris, T. Sun, L. Gregoratti, M. Dalmiglio, and M. Kiskinova *Initial Stages of Oxidation on Graphitic Surfaces: Photoemission Study and Density Functional Theory Calculations* J. Phys. Chem. C 113, 9009 (2009)
25. S. Colussi, A. Gayen, M. Farnesi Camellone, M. Boaro, J. Llorca, S. Fabris, and A. Trovarelli *Nanofaceted Pd-O Sites in Pd-Ce Surface Superstructures Boost Activity in catalytic Combustion of Methane* Angew. Chem. Int. Ed. 48, 8481 (2009)
26. M. Farnesi Camellone and S. Fabris *Reaction Mechanisms for the CO Oxidation on Au/CeO2 catalysts: Activity of Substitutional Au3+/Au+ Cations and Deactivation of Supported Au+ Adatoms* J. Am. Chem. Soc. 131, 10473 (2009)
27. P. Giannozzi et al., " QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials", J. Phys. Cond. Matt. 21, 395502 (2009).
28. X. Wang, M. Shen, J. Wang, and S. Fabris *Enhanced Oxygen Buffering by Substitutional and Interstitial Ni point defects in Ceria: A first-principles DFT+U Study* J. Phys. Chem. C 114, 10221 (2010)
29. A. Wade, S. Lizzit, L. Petaccia, A. Goldoni, D. Diop, H. Ustunel, S. Fabris, and S. Baroni *Metallization of the C60/Rh(100) interface revealed by valence photoelectron spectroscopy and density functional theory calculations* J. Chem. Phys. 132, 234710 (2010)
30. Y. Wang, S. Fabris, G. Costantini, and K. Kern *Tertiary chiral domains assembled by achiral metal-organic complexes on Cu(110)* J. Phys. Chem. C 114, 13020 (2010)
31. L. Szabova, M. Farnesi Camellone, M. Huang, V. Matolin, "Thermodynamic, electronic and structural properties of Cu/CeO$_2$ surfaces and interfaces from first-principles DFT+U calculations", submitted
32. T. Sun, S. Fabris, and S. Baroni, "Surface precursors and reaction mechanisms for the thermal reduction of graphene oxide", submitted
33. S. Piccinin and S. Fabris, "First principles study of water oxidation catalyzed by a tetraruthenium-oxo core within polyoxometalate ligands", submitted