Curriculum Vitae

STEFANO FABRIS

Date of birth: 12 March 1973, Trieste (Italy)
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Professional experience

2008-present	Research staff member, DEMOCRITOS Simulation Center, CNR-IOM Institute, Trieste, Italy;
2004-2008	Tenure-track researcher, DEMOCRITOS Simulation Center, INFM and CNR. *Tenured in 2008;*
2003-2004	Postdoctoral research fellow, INFM-CNR DEMOCRITOS, Trieste, Italy;
2000-2002	Postdoctoral research fellow, Max-Planck-Institut für Metallforschung, Stuttgart, Germany.

Education

2000	Ph.D. degree in physics, Queen's University of Belfast (Prof. M. W. Finnis), UK;
1998	Degree in Materials Science and Engineering, University of Trieste, Italy. 110/100 cum laude.

Management experience

2014-present	Director of the CNR-IOM DEMOCRITOS Simulation Center, Trieste, Italy (www.democritos.it);
2005-2013	Head of the theory group@ELETTRA synchrotron facility (www.democritos.it/the-group).

Awards and distinctions

2016	Shortlisted and ranked second for the CECAM directorship (www.cecam.org)
2016	Honorary Hans Fischer Fellow - Institute for Advanced Studies - Technische Universität München
2015	Friedrich W. Bessel ***research award - Alexander von Humboldt foundation***;
2015	Chinese Academy of Science, President's International Fellowship Initiative;
2014	*Abilitazione nazionale* as associate professor in chemistry (sectors 03/B1 and 03/A2);
2014	*Abilitazione nazionale* as associate professor in theoretical condensed matter physics (sector 02/B2);

Scientific production and activity

- 73 scientific papers published in international journals and refereed conference proceedings: 1 Science, 1 Nature Materials, 1 Nature Comm,1 PNAS, 3 J Am Chem Soc, 3 Phys Rev Lett, 3 Nano Lett, 2 Angew Chem Int Ed, 1 ACS Nano, 2 J Phys Chem Lett, 16 J Phys Chem A-C, 3 J Chem Phys, 11 Phys Rev B, and others. Full list in ANNEX VI;
- 10000+ citations, H-index 29 (source Google Scholar, August 2016);
- 57 invited talks at international conferences (including 2 ACS meetings, 1 MRS meeting, 1 ECOSS, ..). ANNEX II;
- Director/organizer of 12 scientific conferences&workshops (including CECAM, Psi-K). ANNEX IV.

Scientific interests

Keywords: Computational materials science (from electronic structure to atomistic modelling); Nanostructured materials for artificial photosynthesis, water splitting, hydrogen production/purification and fuel cells; Surface chemistry and heterogeneous catalysis; Defect chemistry of materials; Surface-supported organic and metal-organic nanostructures; Multiscale computational methods; Computational spectroscopy and microscopy.

Funding ANNEX V

Principal Investigator, scientist in charge, coordinator

10 M€	EU H2020-INFRAIA-2014/2015 - *Nanoscience foundries and fine analysis for Europe*	2015-2019;
3.9 M€	EU FP7-NMP-2012 - *Design of thin-film nano catalysts for on-chip fuel cell technology.*	2013-2016;
100 K€	EU FP7-PEOPLE-IRG-2008 - *Water splitting Catalysts for Artificial Photosynthesis.*	2009-2013;
300 K€	Convenzione quadro CNR- Sincrotrone Trieste s.r.l (ELETTRA).	2007-2013;
40 K€	PRIN - *Controlling the structure&function of metallorganic nanostructures on metal surfaces;*	2010-2013;
78 K€	FVG regional grant: *Nanocatalysis on carbon-based materials.*	2008-2010.

Participant:

- FP7-PEOPLE-COST-2011 - CM1104 *Reducible oxide chemistry, structure and functions* 2013-2015;
- PRIN: GRAF *Frontiere della ricerca sul grafene: comprensione e controllo di funzionalità avanzate* 2013-2016;
- FP7-INFRA-2007-2.1.1: NFFA - Nanoscience Foundries and Fine Analysis 2011-2013;

PI and in computational grants (last 4 years only):
>55 M hours on HPC infrastructures (PRACE - Partnership for Advanced Computing in Europe www.prace.eu)

10/10/2016

Teaching experiences

2010-present	PhD course electronic structure & materials science, SISSA, Trieste, Italy;
2015-2016	PhD course, *Computational Surface Science and Catalysis*, University of Padova, Italy. ANNEX I;
2010-2011	Undergraduate course, Computational materials science, University of Trieste, Italy. ANNEX I;
2006-present	Supervisor of 6 PhD, 3 MSc students, 13 postdoctoral fellows. ANNEX II;
2004-present	16 invited lectures at schools&workshops in the field of computational materials science. ANNEX III;
2000-2002	Teaching assistant, MSc course, "*Electronic structure of condensed matter*", University of Stuttgart;

Research visits

2015-2016	Technische Universität München (*fellowship*)
2013	National Institute for Materials Science, Tsukuba, Japan (*Invited*);
2011	CECAM, Centre Européen de Calcul Atomique et Moléculaire, Lausanne, CH (*Invited*);
2010	Molecular Foundry, Lawrence Berkeley National Lab., Berkeley, USA;
2005	Max-Planck-Institut für Festkörperforschung, Stuttugart, Germany (*travel fellowship*);

Other professional activities

- Member of PhD and Master examination committees for: Humboldt University, University of Lyon, Aarhus University; King's College of London; SISSA, University of Ljubljana; Charles University of Prague; Università Ca' Foscari, Università di Trieste;
- Associate Editor - Journal of Materials for Renewable and Sustainable Energy - Springer Ed. (2012-present);
- Member of the steering board of the Users Forum Partnership for Advanced Computing in Europe (PRACE);
- Expert reviewer for international funding agencies: European Research Council (ERC); US Air Force Office of Scientific Research (AFOSR); US Department of Energy (DOE); Swiss National Science Foundation (SNFS); Austrian Science Fund (ASF); Research Grants Council of Hong Kong; National Science Centre – Poland;
- Expert reviewer for scientific supercomputing centers: Partnership for Advanced Computing in Europe (PRACE), CINECA Italian SuperComputing Resource Allocation; Swiss Center for Scientific Computing of the ETH Zurich.
- Referee for international journals: Nature Chemistry, Nature Communications, Physical Review Letters, J. Am. Chem. Soc., Physical Review B, Applied Physics Letters, Advanced Functional Materials, Journal of Physical Chemistry, Journal of Chemical Physics, Phys. Chem. Chem. Phys., Surface Science, Catalysis Comm, ...

Selected publications

1. 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) [710 citations]
2. M. Farnesi Camellone, A. Tovt, N. Tran, F. R. Negreiros, I. Matolínová, J Mysliveček, V. Matolín, S. Fabris
   Creating single-atom Pt-ceria catalysts by surface step decoration
   Nature Comm. 7, Article number: 10801 (2016) [9]
3. Y. Lykhach, S. M. Kozlov, T. Skala, A. Tovt, V. Stetsovych, N. Tsud, F. Dvorak, V. Johanek, A. Neitzel, J. Myslivecek, S. Fabris, V. Matolin, K. M. Neyman, J. Libuda
   Counting Electrons on Catalyst Nanoparticles
   Nature Materials 15, 284–288 (2016) [14]
4. T. Sun and S. Fabris
   Mechanisms for oxidative unzipping and cutting of graphene
   Nano Letters 12, 17 (2012) [77]
5. 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) [297]
6. M. Farnesi Camellone and S. Fabris
   Reaction Mechanisms for the CO Oxidation on Au/CeO2 catalysts
   J. Am. Chem. Soc. 131, 10473 (2009) [162]
7. 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) [111]
8. R. Larciprete, S. Fabris, T. Sun, P. Lacovig, A. Baraldi, and S. Lizzit
   Dual path mechanism for the thermal reduction of graphene oxide
   J. Am. Chem. Soc. 133, 17315 (2011) [176]
9. M. Huang and S. Fabris
   CO adsorption and oxidation on ceria surfaces from DFT+U calculations
   J. Phys. Chem. C **112**, 8643 (2008). [151]
10. *QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials*
    J. Phys. Cond. Matt. **21**, 395502 (2009). [6824]

ANNEX I
TEACHING

Graduate and Postgraduate courses

1. ***International School for Advanced Studies – SISSA***. 2010-present
   Electronic structure course in the PhD program of condensed matter
   Introductory lectures on the physical chemistry of materials
   Topical lectures and computer laboratory on advanced simulation methods for modeling nanostructured materials
   Topical lectures on Simulation methods for surface science, surface reactions & catalysis and activated processes

2. ***University of Padova***. 2015-2016
   PhD program of Materials science and engineering
   Computational Surface Science and Catalysis

3. ***University of Trieste***. 2010-2011
   Titolare del corso di laurea specialistica in Ingegneria dei Materiali ING-IND/22
   Modellizzazione su base micro e nano strutturale

Lectures and hands-on laboratories at schools and workshops

4. ***Workshop on Materials Science for Energy Storage***, Abdus Salam International Centre for Theoretical Physics (ICTP), Italy, 11-15/05/2015. *Lectures on "Energy conversion by catalytic interfaces".*

5. ***From the chemical bond to the chemical reactor: Computational and materials challenges in gas conversion technologies***, CECAM Workshop, JNCASR Bangalore (India), 25-28/8/2014.
   Two lectures and a computer lab on "Modelling chemical reactions and activated events at materials surfaces".

6. ***Computer modeling of materials at the nanoscale***, The University of Tokyo, 23-26/4/2014
   Two lectures and a computer lab on "Simulation techniques for exploring potential energy surfaces".

7. ***CECAM/SISSA summer school on atomistic modeling techniques***, SISSA, Trieste - 25/7/2013
   Two lectures and a computer lab on i) Computational theories and algorithms for the simulation of activated events; ii) Insight into materials properties from DFT calculations - post processing data.

8. ***Summer school for the PhD program of the University of Trieste*** "La filiera dell'energia rinnovabile tra sole, idrogeno e smart grid" - Sesto – 24-28/6/2013
   One lecture on fundamentals of computational materials modeling and on its applications to renewable-energy technologies.

9. ***ICTP Workshop on Advances in Materials Science*** (KWAMS'13) – Khartoum – 19-31/1/2013
   Three lectures and four computer laboratories on fundamentals and implementations of density functional theory for the simulation of materials properties.

10. ***ICTP Workshop on Numerical Methods for Materials Science Related to Renewable Energy Applications***, International Center for Theoretical Physics, Trieste - 26-30/11/2012
    Two lectures and a computer laboratory on computational catalysis and its applications to renewable-energy materials and processes.

11. ***Joint ICTP-TWAS II Latin American School on Computational Materials Science for Energy and Environmental Applications***, Santo Andrè, Brazil - 5-16/9/2011
    Two lectures and two computer laboratories on fundamentals and implementations of density functional theory for the simulation of materials properties.

12. ***CECAM/SISSA summer school on atomistic modeling techniques***, SISSA, Trieste - 5-23/7/2010
    Two lectures on elementary electronic structure theory and its implementation into advanced computer codes.

13. ***IARS Frontiers workshop: Advanced School and International Conference on DFT and its Applications in Nanosciences***, Marmaris Turkey - 19-29/10/2009
    Three lectures and two computer laboratories on fundamentals of density functional theory and on its application to surface science.

14. ***Latin American School on Computational Materials Science***, Universidad Andrés Bello, Santiago del Chile – 19-30/1/2009
    Two lectures and two computer laboratories on fundamentals and implementations of density functional theory for the simulation of materials properties.

15. ***Winter School on Applications of Computer Simulation and Modelling in Contemporary Solid State Physics and Nanotechnology***, Marmaris, Turkey - 28/1-6/2/2008
Three lectures and two computer laboratories on fundamentals of density functional theory and on its application to surface science.

16. ***CECAM workshop "Simulating matter at the nano-scale using density-functional theory, pseudopotentials and plane waves***", Lyon, France - 13-17/11/2006
One lecture and two computer laboratories on the implementation of density functional theory in a plane-wave and pseudo potential framework, and on its use to model chemical reactions and other activated events.

17. ***Tutorial on the ab-initio simulation of the electronic, structural and dynamical properties of materials*** - Università degli Studi di Cagliari - 29-30/9/2005
Two computer laboratories on the use and implementation of density functional theory in a plane-wave and pseudo potential framework.

18. ***Tutorial on the ab-initio simulation of the electronic, structural and dynamical properties of materials*** - International Center for Theoretical Physics, Trieste - 17-21/1/2005
Two computer laboratories on the use and implementation of density functional theory in a plane-wave and pseudo potential framework.

19. ***Tutorial on the ab-initio simulation of the electronic, structural and dynamical properties of materials*** - Consorzio Interuniversitario per il Calcolo Avanzato, CINECA, Bologna - 1-5/3/2004
Two computer laboratories on the use and implementation of density functional theory in a plane-wave and pseudo potential framework.

20. ***Winter College on Numerical Methods in Electronic Structure Theory*** - International Center for Theoretical Physics ICTP, Trieste - 16-31/1/2003
One lecture on numerical algorithms for matrix diagonalization and for minimization problems. Three computer laboratories on the use and implementation of density functional theory in a plane-wave and pseudo potential framework.

ANNEX II
SUPERVISION AND TRAINING

PhD and MSc students

- Guido Fratesi, MSc student, International School for Advanced Studies SISSA, 2004.
- Adriano Mosca Conte, PhD student, International School for Advanced Studies SISSA, Thesis title: *Quantum mechanical modeling of nano magnetism: new tools based on Density-Functional theory with case applications to solids, surfaces, wires, and molecule*, 2008;
- Changru Ma, PhD student, International School for Advanced Studies SISSA, Thesis title: *Modeling Ru-based molecular catalysts for water oxidation*, 2012;
- Lucie Szabova, MSc student, Department of Surface and Plasma Science, Charles University of Prague, Thesis title *Ab initio study of Cu-Ce-O interfaces*, 2008;
- Lucie Szabova, PhD student, Department of Surface and Plasma Science, Charles University of Prague, Thesis title: *Ab initio study of ultrathin ceria films on Cu(111)*, 2013;
- Tommaso Francese, Master student, Università Ca' Foscari, Venezia, Thesis title: *Ab initio simulation and investigation of a novel Ta-doped Zirconia material*, 2014;
- Michal Fecik, PhD student, International School for Advanced Studies SISSA, 2014;
- Nguyen Dung Tran, PhD student, International School for Advanced Studies SISSA, 2014;
- Luca Dietz, PhD student, Politecnico di Milano, 2014.

Postdoctoral fellows

- Min Huang, INFM DEMOCRITOS Simulation Center, 2005-2007. Now assistant professor at Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan 430071, China;
- Hande Hüstünel, INFM DEMOCRITOS, 2005-2006. Now assistant professor at Department of Physics, Middle East Technical University.
- Matteo Farnesi Camellone, INFM DEMOCRITOS Simulation Center, 2007-2009. Now staff researcher at CNR-IOM DEMOCRITOS;
- Tao Sun, International School for Advanced Studies SISSA, 2008-2011. Now associate professor at University of Chinese Academy of Sciences, Beijing, China;
- Simone Piccinin, CNR-IOM DEMOCRITOS, 2009. Now permanent staff researcher at CNR-IOM DEMOCRITOS;
- Xiaoliang Hu, CNR-IOM DEMOCRITOS and SISSA, 2010-2012. Now postdoctoral research fellow at École polytechnique fédérale de Lausanne, EPFL;
- Sara Fortuna, CNR-IOM DEMOCRITOS, 2010-2012. Now postdoctoral research fellow at Università degli Studi di Udine;
- Sara Furlan, International School for Advanced Studies SISSA, 2012-2014. Now postdoctoral research fellow at Università degli Studi di Trieste;
- Karolina Kwapien, CNR-IOM DEMOCRITOS, 2012-2014;
- Praveen Surendram Chandramati, CNR-IOM DEMOCRITOS, 2012-2014. Now research fellow at ETH Zurich;
- Fabio Ribeiro, CNR-IOM DEMOCRITOS, 2012-2014;
- Matteo Farnesi Camellone, CNR-IOM DEMOCRITOS, 2014-present, researcher;
- Luigi Bagolini, CNR-IOM DEMOCRITOS, 2015-present.

Visiting fellows

- Xinquan Wang, PhD student at the School of Chemical Engineering and Technology, Tianjin University. Training in DFT simulations on oxide materials and co-supervisor of PhD Thesis. 3 months visit, October-December 2008;
- Yansun Yao, PhD student at the Physics Department, University of Saskatchewan, Canada. Training in the ab-initio simulation of X-ray photoemission spectroscopy. 2 months visit, March-April 2008;
- Sebastian Pehan, PhD student at the J. Stefan Institute, Ljubljana, Slovenia. Training in ab-initio and empirical modeling of organic molecules in solution. 2 months visit, April-May 2010;
- Masoud Nahali, PhD student at the Sharif University of Technology, Teheran, Iran. Training in the ab-intio simulation of oxidation processes on graphitic substrates. 6 months visit, August 2011-Janusary 2012;
- Sergey Kozlov, PhD student at University of Barcelona, March-May 2014.
- Tommaso Francese, PhD student at University of Barcelona, June 2016

ANNEX III
INVITED TALKS AND SEMINARS

Invited talks at international conferences and workshops

1. ***X International Conference Mechanisms of Catalytic Reactions*** – Kaliningrad, Russia 2-6/10/2016
2. ***College on Multiscale Computational Modeling of Materials for Energy*** –International Centre for Theoretical Physics (ICTP), Italy 4-15 July, 2016
3. ***Joint MCC-UKCP-EPCC Workshop on Ab initio Periodic Codes*** -- STFC Daresbury Laboratory (UK), 19-22/2/2016
4. ***American Chemical Society Fall Meeting*** – Boston, USA – 16-20/8/2015
5. ***International Conference on Chemical Bonding, ICCB*** – Kauai, USA – 2-6/7/2015
   Title: *Bonding and reactivity at catalytic interfaces: Modelling novel fuel-cell electrodes from ideal to realistic reaction environments*
6. ***National Conference on Condensed Matter Physics - FISMAT 2015*** – Palermo, Italy – 28/9-2/10/2015
7. ***Workshop on Materials Science for Energy Storage -*** ICTP, Trieste, Italy – 11-15/5/2015
   Title: *Energy conversion by catalytic interfaces: Ab-initio modelling of novel electrodes from ideal to realistic reaction environments*
8. ***Energy&Materials Nanotechnology Meeting- EMN 2015*** – Istanbul, Turkey–
9. ***Materials Research Society Fall Meeting*** – Boston – 30/11-5/12/2014
   Title: *Reducing the Pt content in fuel-cell electrodes Reactivity and stability of Pt/CeO2 nanomaterials from first-principles modelling*
10. ***7th International Conference on Materials for Advanced Technologies*** - Singapore - 30/6-5/7/2013
    Title: *Computational Modeling of Nanostructured Materials for Solar-driven Fuel Production*
11. ***4th Regional Symposium on Electrochemistry of South-East Europe*** (RSE-SEE4) - Ljubljana - 26-30/05/2013
    Title: *Computational Modeling of New Materials for Electrochemical Solar-to-fuel Energy Conversion*
12. ***ICTP Workshop on Advances in Materials Science*** (KWAMS'13) – Khartoum – 19-31/1/2013
    Title: *Surface-supported Metal Clusters: Insight from Computational Modeling*
13. ***UNESCO Advanced Workshop on Solar Energy Conversion*** - Bucharest - 21-24/5/2012
    Title: *Computation al Modeling of New Materials for Solar-driven Fuel Production*
14. ***NANOENERGETICS: Theoretical and Experimental Approaches*** - ICTP Trieste - 15-16/11/2011
    Title: *Novel Materials for Solar Energy Conversion and Storage: Insight from first-principles modeling*
15. ***COST ACTION MP0901, Designing novel materials for nanodevices: From Theory to Practice*** – ICTP Trieste – 9-11/11/2011
    Title: *Atomistic mechanisms for oxidative unzipping and cutting of graphene*
16. ***American Chemical Society meeting***, Denver, USA - 28/08-1/09/2011
    Title: *Reaction mechanism and thermodynamics of efficient water oxidation catalyzed by tetraruthenium-oxo clusters in solution*
17. ***International Atomic Energy Agency Advanced School*** - Development and characterization of materials for hydrogen-based energy systems: role of nuclear technology, ICTP Trieste - 13-18/6/2011
    Title: *Computational modeling of catalytic materials for Hydrogen-based technologies*
18. ***Workshop of the PhD in Nanotechnology*** - Università di Trieste, 20-23/9/2011
    Title: *Computational Materials Science for Energy Conversion and Storage*
19. ***ICTP-TWAS II Latin American Workshop*** on Computational Materials Science for Energy and Environmental Applications, Santo Andrè, Brazil - 5-16/9/2011
    Title: *Computational modeling of catalytic materials for energy and environmental applications*
20. ***CECAM workshop*** on "Understanding structure and functions of reducible oxide systems-a challenge for theory and experiment", Zaragoza, Spain - 20-23/06/2011
    Title: *Catalytic activity of metal clusters and substitutional ions at reducible oxide surfaces*

21. ***CECAM workshop*** on "Charge and Spin Transport in Chemically Modified Graphene-Based Materials", Barcelona, Spain - 7-8/4/2011
    Title: *Thermal evolution of oxidized graphene*

22. ***Workshop su Fisica della Materia e Scienza dei Materiali Computazionali***, CNR, Rome - 21-22/2/2011
    Title: *Computational materials science for energy conversion and storage*

23. ***Energy Materials Workshop***, Thomas Young Center, London - 7-9/9/2010
    Title: *Ab initio modeling of homogeneous catalysts for water oxidation*

24. ***CECAM workshop*** "Electronic-structure challenges in materials modeling for energy applications", Lausanne - 1-4/6/2010
    Title: *Catalytic activity of gold nanoclusters supported by cerium oxide*

25. ***I International workshop on cerium oxide***, Modena, Italy - 23-25/6/2010
    Title: *Modelling the reactivity of ceria-supported metal nanoparticles with DFT+U calculations*

26. ***US Department of Energy meeting, Discovery in Basic Energy Science***: The role of Computing at the Extreme Scale Washington, USA - 13-15/08/2009
    Title: *Computational materials science for energy conversion and storage*

27. ***Latin American School on Computational Materials Science***, Santiago, Chile - 19-30/1/2009
    Title: *Understanding the structure and function of self-assembled organometallic nanomaterials by computer modeling*

28. ***Psi-K workshop*** on "Ab Initio Modelling in Applied Biosciences: Structure, Dynamics and Function", Uppsala University, Sweden 11-12/12/2008
    Title: *Concerted catalytic action of di-iron centers dissociates O2*

29. ***22nd conference of the European Physical Society***, Rome, Italy - 25-29/8/2008
    Title: *Understanding the structure and function of self-assembled organometallic nanomaterials by computer modeling*

30. ***2nd International Workshop on Materials Science and Nano-Engineering***, Awaji Island, JAPAN - 1-5/12/2007
    Title: *Properties of surface-supported nanomagnets from relativistic DFT calculations*

31. ***American Chemical Society Fall Meeting***, Boston, USA - 19-23/8/2007
    Title: *Oxygen buffering at reducible oxide surfaces: Interplay between vacancies, electron localization, and adsorbate mobility on ceria*

32. ***24th European Conference on Surface Science ECOSS 24***, Paris - 4-8/9/2006
    Title: *Oxygen buffering at reducible oxide surfaces: interplay between vacancies, electron localization, and adsorbate mobility on ceria*

33. ***Colloquium on "Nanostructured Oxide Surfaces"***, Dipartimento di chimica, Università di Torino, Italy - 23-24/3/2006
    Title: *Modeling the surface chemisrty of Cerium Oxide using Density Functional Theory*

34. ***European Science Foundation EUROCORES workshop*** "Functional molecular nanostructures", Kloster Irsee, Germany - 26-29/4/2006
    Title: *Insight into the electronic and magnetic properties of Tb Double- Decker molecular magnets*

35. ***ELETTRA Workshop*** on "Computer Simulation of Surface and Interface Phenomena", ICTP, Trieste - 14-16/12/2005
    Title: *Oxygen vacancies and electron localization at reducible oxide surfaces*

36. ***High-Performance Computing Transnational Access Meeting***, High Performance Computing Center Stuttgart (HLRS) University of Stuttgart - 21-24/9/2005
    Title: *First-principles calculations of metal-organic nanostructures*

37. ***MMD Matter, Materials, and Devices Meeting***, Genova - 22-25/6/2005
    Title: *Taming multiple valency with density functionals: the case of reduced ceria*

38. ***ECSAC Conference*** "Nanosciences and Nanotechnology" - 6-10/9/2004
    Title: *The atomistic puzzle of a molecular necklace: the case of trimesic acid on Cu(111)*

Invited seminars

39. Colloquium at Friedrich-Alexander-Universitaet Erlangen-Nuernberg – 27/1/2016

40. Colloquium at ***Technische Universitaet Muenchen*** – 9/11/2015

41. Colloquium at ***Beijing Computational Science Research Center*** (CSRC) – 9/10/2015

42. Colloquium at ***The Abdus Salam International Centre for Theoretical Physics*** – 15/4/2015
Title: *Combining electronic-structure and enhanced-sampling molecular dynamics methods to model fuel-cell electrodes in working conditions*

43. Keynote seminar at the opening day of the Academic Year 2014-2015, Doctoral school of Engineering ***Università degli Studi di Trento*** – 4/3/2015 – Host: Prof. Paolo Scardi
Title: *Design Guidelines of Materials for renewable-energy technologies from First Principles*

44. ***Università degli Studi di Brescia*** – 16/12/2014 – Host: Prof. Alberto Salvadori
Title: *Computational Modeling of New Materials for Solar-driven fuel production*

45. ***University of Tokyo***, Japan – 28/8/2013 – Host: Tsuneyuki
Title: *Computational Modeling of New Materials for Electrochemical Solar-to-Fuel Energy Conversion*

46. ***National Institute for Materials Science***, Tsukuba, Japan – 23/8/2013 – Host: Y. Tateyama
Title: *Computational Modeling of New Materials for Electrochemical Solar-to-Fuel Energy Conversion*

47. ***University of the Basque Country and nanoGUNE***, San Sebastian - 12/2/2013 – Host: A. Rubio
Title: *Unifying Concepts in Water Oxidation Catalysis: Surface mechanisms replicated at molecular sites*

48. Institute of Materials Chemistry, ***Vienna University of Technology***, Austria - 21/3/2012 - Host: G. Rupprechter
Title: *Catalytic activity of metal clusters and substitutional ions at reducible oxide surfaces*

49. ***Josef Stefan Institute***, Ljubljana, Slovenia - 7/2/2012 - Host: A. Kokalj
Title: *Heterogeneous catalysts based on transition metals and reducible oxides: Insight from first-principles calculations*

50. Colloquium at ***Technical University of Munich***, Deutschland - 21/11/11 - Host: F. Esch
Title: *Catalytic activity of metal clusters and substitutional ions at reducible oxide surfaces*

51. ***University College Cork***, Ireland - 28/9/11 - Host: M. Nolan
Title: Catalytic activity of metal clusters and substitutional ions at reducible oxide surfaces

52. ***Center for Functional Nanomaterials***, Brookhaven National Laboratory, USA - 3/8/2010 - Host: Mark S Hybertsen
Title: *Catalytic activity of Au nanoclusters supported by Cerium oxide*

53. ***Molecular Foundry, Lawrence Berkeley National Laboratory***, Berkeley, USA - 28/7/2010 - Host: Jeffrey Neaton
Title: *Catalytic activity of Au nanoclusters supported by Cerium oxide*

54. ***Charles University, Prague***, Check Republic - 15/9/2009 - Host: V. Matolin
Title: *Structure and reactivity of metal nanoparticles supported by ceria surfaces*

55. ***Tianjin University***, China - 18/09/2009 – Host:
Title: *Reactivity and deactivation of metal nanoparticles suppported by reducible oxides: The case of the Au/CeO2 catalyst*

56. ***Charles University of Prague***, Check Republic - 16/05/2007 – Host: Vladimir Matolin
Title: *Oxygen buffering at reducible oxide surfaces:interplay between vacancies, electron localization, and adsorbate mobility*

57. ***Max-Planck Institut fuer Festkoerperforschung***, Stuttgart - 17/4/2004 – Host: K. Kern
Title: *Structure and chemical reactivity of reduced ceria surfaces*

ANNEX IV
ORGANIZATION OF CONFERENCES & WORKSHOPS

1. ***CECAM workshop -- Interface processes in photochemical water splitting: Theory meets experiment***
   27-30/09/2016, EPFL, Lausanne, CH

2. ***CECAM workshop - From the chemical bond to the chemical reactor: Computational and Materials challenges in gas conversion technologies***
   25-28/8/2014, International Centre for Materials Science, Bangalore, India
   Directors: S. Fabris, S. Narasimhan, S. Piccinin, L. Spanu
   http://www.democritos.it/bangalore2014

3. ***Workshop on Material Challenges in Devices for Solar Fuel Production and Employment***
   19-23/5/2014, International Center for Theoretical Physics, Trieste,
   Organizer(s): T. Bligaard, N. Bonini, A. De Vita, S. Fabris, R. Gebauer, S.C. Roy, N. Seriani.
   http://cdsagenda5.ictp.it/full_display.php?email=0&ida=a13198

4. ***CECAM Conference Energy from the Sun: Computational Chemists and Physicists Take up the Challenge***
   10-14/09/2012, Chia Laguna, Sardinia, Italy.
   Directors: W. Andreoni, V. Barone, S. Fabris, G. Galli, A. Mattoni;
   http://www.cecam.org/workshop-820.html

5. ***ICTP School on Numerical Methods for Materials Science Related to Renewable Energy Applications***
   26-30/11/2012, International Center for Theoretical Physics, Trieste, Italy
   Directors: F. De Angelis, S. Fabris, R. Gebauer, N. Seriani
   http://cdsagenda5.ictp.trieste.it/full_display.php?ida=a11191

6. ***CECAM Workshop "Chemical and topological functionalization of graphitic surfaces: open challenges for computational modeling"***
   23-25 April 2012, Centre Européen de Calcul Atomique et Moléculaire – CECAM, Lausanne CH
   Directors: G. Benedek and S. Fabris
   http://www.cecam.org/workshop-786.html

7. ***SISSA-ICTP Workshop on New Materials for Renewable Energy***
   October 2011, International Center for Theoretical Physics, Trieste
   Directors: S. Fabris and R. Gebauer
   http://cdsagenda5.ictp.trieste.it/full_display.php?ida=a10178

8. ***15th Workshop on Computational Physics and Materials Science: Total Energy and Force Methods***
   Jan 2011, International Center of Theoretical Physics (ICTP), Trieste
   Directors: L. Reining, I. Souza, S. Fabris; R. Gebauer
   http://cdsagenda5.ictp.it/full_display.php?agenda_id=3218

9. ***10th ECSAC conference on "Sustainable Energy: Challenges and Opportunities"***
   August 2010, Losinj (Croatia)
   Directors: A. Treleani and S. Fabris
   http://ecsac.ictp.it/ecsac10/index.php

10. ***Psi_k 2010 Conference*** - Symposium *Catalysis from first principles: Energy conversion and storage*, 12-16/11/2010, Berlin (Germany).
    Organizers: T. Bligaard and S. Fabris
    http://th.fhi-berlin.mpg.de/th/Meetings/psik_2010/

11. ***Computer Simulation of Surface and Interface–Phenomena***
    ELETTRA synchrotron laboratory, 15-16 Dec. 2005, Trieste (Italy)
    Organizers: S. Baroni, S. Fabris, A. Goldoni, M. Kiskinova
    http://www.elettra.trieste.it/events/2005/um13/

12. ***Tutorial on Ab-initio simulation of the electronic, structural and dynamical properties of materials***,
    26-30 Sept. 2005, SLACS center of the CNR, Cagliari (Italy);

Organizers: S. Baroni, S. Fabris, P. Giannozzi, P. Ruggerone, A. Satta
http://www.democritos.it/events/espresso-tutorial-2.php

ANNEX V

FUNDING

Principal Investigator and person in charge

EU H2020-INFRAIA-2014/2015 - Nanoscience foundries and fine analysis for Europe
Principal Investigator of CNR unit and Coordinator of Theory Workpackage
Other partners involved: CNR Consiglio Nazionale delle Ricerche, CEA CNRS FR, DESY DE, EPFL CH, ESRF EU FORTH - Hellas EL, ICN2 ES, Juelich Forschungszentrum Juelich GmbH DE, KIT Karlsruhe Institut fuer Technologie DE, Lunds Universitet SE, PRUAB ES, Paul Scherrer Institute CH, STFC Science and Technology Facilities Council UK, Technische Universitaet Graz AT, Technische Universitaet Muenchen DE, Universita` degli Studi di Milano IT, Univerza v Novi Gorici SI, Universidad del Pais Vasco
Total funding: 10 M€
Funding of CNR unit: 260 K€
Funding period: January 2013- December 2016

EU FP7 project - Design of thin-film nano catalysts for on-chip fuel cell technology - FP7-NMP-2012
Principal Investigator of CNR unit
Other partners involved: Charles University of Prague, UNIVERSITAT ERLANGEN NURNBERG, UNIVERSITE DE BOURGOGNE, UNIVERSITAT DE BARCELONA, ThunderNIL srl, L.E.T. optomechanika Praha, SOLVICORE GMBH & CO KG
Total funding: 3.914 K€
Funding of CNR unit: 389 K€
Funding period: January 2013- December 2016

MIUR PRIN 2008 - Controllare la struttura e le funzioni di nanostrutture organiche su superfici metalliche
Principal Investigator of CNR unit *(Responsabile unità operativa CNR)*
Other partners involved: Roma La Sapienza (Capofila); Università degli Studi di Modena;
Total funding: 185 K€
Funding of CNR unit: 40 K€
Funding period: March 2010- February 2013

EU FP7 project Water Splitting Catalysts for Artificial Photosynthesis - FP7-PEOPLE-IRG-2008
Scientist in charge for CNR
Other partners involved: none;
Total funding: 100 K€
Funding period: May 2009 - April 2013

FVG Regional Project "Nanocatalisi su fili e fibre di carbonio" – 473/LAVFOR/2008
Principal Investigator of CNR unit
Other partners involved: SISSA, University of Trieste, University of Udine, Sincrotrone TS, EUROTECH
Total funding: 390 K€
Funding of CNR unit: 78 K€
Funding period: October 2008 - September 2011

Theory@Elettra project
Principal Investigator, head of the research group and person in charge of the agreement "*Convenzione quadro tra CNR-IOM, protocollo N. 13985 del 15/12/2006 e rinnovo 1145 del 22/06/2010*"
Other partners involved: SISSA
Total funding: 300 K€
Funding period: December 2006 - June 2013

Participant

Nanoarchitectonic control of efficient oxidation process on surface/interface for next-generation catalysts and fuel cell – Japanese National Institute for Materials Science
Participant
Other partners involved: Charles University of Prague;

Total funding: 5.000 KYen;
Funding period: January 2014 - December 2016

EU FP7 COST Action CM1104 Reducible oxide chemistry, structure and functions -FP7-PEOPLE-COST
Participant to the Working Group 3 - REACTIVITY
Other partners involved: large EU network with more than 10 participants;
Total funding: the project funds collaborative visits and participation to meetings and workshops;
Funding period: April 2012 - March 2015

MIUR PRIN 2010 - GRAF Frontiere della ricerca sul grafene: comprensione e controllo di funzionalità avanzate
Participant to the SISSA unit
Total funding: 1.565.550 K€
Funding period: March 2010- February 2013

EU FP7 project - NFFA - Nanoscience Foundries and Fine Analysis- FP7-INFRA-2007-2.1.1
Participant to CNR unit
Other partners involved: STFC- SCIENCE AND TECNOLOGY FACILITIES COUNCIL;
PSI - PAUL SCHERRER INSTITUT;
CSIC-CNM - CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFCAS
OEAW- OESTERREICHISCHE AKADEMIE DER WISSENSCHAFTEN
Total funding: 1.800 K€
Funding of CNR unit: 703 K€
Funding period: June 2008- May 2011

Computational grants

- ***PRACE 2013 Tier 0***, *Ab-initio modeling of novel catalysts for fuel-cell electrodes under operative conditions*
  35 M core/hours. PI;
- ***PRACE 2012 Tier 0***, *Shedding light on the catalytic core of artificial leaf technologies*
  35 M core/hours. PI;
- ***ISCRA 2012*** - *First-principles investigation of supported Au clusters for heterogeneous catalysis*
  4.6 M core/hours. Co-PI;
- ***ISCRA 2012*** - *Accurate simulations of the photoemission spectra of metal supported metal-phthalocyanine self-assemblies*
  3.6 M core/hours. Participant;
- ***PRACE 2011*** - *Multicenter cobalt-oxo cores for catalytic water oxidation*
  4.8 M core/hours. Co-PI
- ***ISCRA 2010*** - *Functionalized carbon nanotubes for artificial photosynthesis*
  1 M core/hours. Co-PI
- ***DEISA/DECI 2010*** - *Water splitting catalysts for artificial photosynthesis*
  1.5 M/core/hours. Co-PI
- 2003-2010: Coordinator of 8 national HPC projects on CINECA supercomputers in the INFM Parallel Computation Initiative.

ANNEX VI
PUBLICATIONS

10000+ citations, H-index=29 (source Google Scholar, August 2016)
https://scholar.google.it/citations?user=t7stXLgAAAAJ&hl=it

Submitted

1. Tran Nguyen Dung, Matteo Farnesi Camellone, and Stefano Fabris
Methanol Oxidation at Pt/Ceria Surfaces: Probing Reactivity of Ionic and Metallic Pt sites with DFT+U Calculations
Submitted to ACS Catalysis

International refereed journals

2. Matteo Farnesi Camellone, Fabio Negreiros, Lucie Szabova, Yoshitaka Tateyama, Stefano Fabris
Catalytic proton dynamics at the water/solid interface of ceria-supported Pt clusters
Journal of the American Chemical Society 138, 11560 (2016)
3. M. Farnesi Camellone, A. Tovt, N. Tran, F. R. Negreiros, M. Vorokhta, T. Skála, I. Matolínová, J Mysliveček, V. Matolín, S. Fabris
Creating single-atom Pt-ceria catalysts by surface step decoration
Nature Comm. 7, Article number: 10801 (2016)
4. Y. Lykhach, S. M. Kozlov, T. Skala, A. Tovt, V. Stetsovych, N. Tsud, F. Dvorak, V. Johanek, A. Neitzel, J. Myslivecek, S. Fabris, V. Matolin, K. M. Neyman, J. Libuda
Counting Electrons on Catalyst Nanoparticles
Nature Materials 15, 284–288 (2016)
5. Y. Lykhach, A. Figueroba, M. Farnesi Camellone, A. Neitzel, T. Skála, F. R. Negreiros, M. Vorokhta, N. Tsud, K. C. Prince, S. Fabris, K. M. Neyman, V. Matolín, J. Libuda
Reactivity of Atomically Dispersed Pt2+ Species towards H2: Model Pt−CeO2 Fuel Cell Catalyst
Physical Chemistry Chemical Physics 18, 7672 (2016)
6. Tao Sun, Xinxin Yao, and Stefano Fabris
Effects of Thermal Electronic Excitations on the Diffusion of Oxygen Adatoms on Graphene
J. Phys. Chem. A, (2016)
7. C. Struzzi, C.S. Praveen, M. Scardamaglia, N.I. Verbitskiy, A.V. Fedorov, M. Weinl, M. Schreck, A. Grüneis, S. Piccinin, S. Fabris, and L. Petaccia
Controlled thermodynamics for tunable electron doping of graphene on Ir(111)
Phys. Rev. B 94, 085427 (2016)
8. K. Ševčíková, L. Szabová, M. Kettner, P. Homola, N. Tsud, Stefano Fabris, V. Matolín
Experimental and Theoretical Study on the Electronic Interaction Between Rh Adatoms and CeOx Substrate in Dependence on a Degree of Cerium Oxide Reduction
J. Phys. Chem. C 120, 2468 (2016)
9. Fabio Ribeiro Negreiros, Matteo Farnesi, and Stefano Fabris
Temperature effects on the dissociation of hydrogen on ceria surfaces
J. Phys. Chem. C 119, 21567 (2015)
10. C. S. Praveen, Simone Piccinin, and Stefano Fabris
Adsorption of alkali adatoms on graphene supported by Au/Ni(111)
Physical Review B 92, 075403 (2015).
11. Simone Piccinin and Stefano Fabris
Water Oxidation by Ru-Polyoxometalate Catalysts: Overpotential Dependency on the Number and Charge of the Metal Centers
Inorganics 3, 374 (2015).
12. A. Fedorov, C.S. Praveen, N.I. Verbitskiy, D. Haberer, D. Usachov, D. V. Vyalikh, A. Nefedov, C. Woll, L. Petaccia, S. Piccinin, K. Mullen, H. Sachdev, M. Knupfer, B. Büchner, S. Fabris, and A. Gruneis
Efficient gating of epitaxial boron nitride monolayers by ionic functionalization
Physical Review B 92, 125440 (2015).
13. Lucie Szabova, Yoshitake Tateyama, Vladimir Matolin, and Stefano Fabris
Water adsorption and dissociation at metal-supported ceria thin films: Thickness and interface-proximity effects studied with DFT+U calculations
J. Phys. Chem. C 119, 2537 (2015).

14. Changru Ma, Stefano Fabris, Alessandro Laio and Simone Piccinin
QMMMW: A wrapper for QM/MM simulations with Quantum ESPRESSO and LAMMPS
Computer Physics Communications (2015).

15. Fabio N. Ribeiro and Stefano Fabris
Role of cluster morphology in the dynamics and reactivity of sub-nm Pt clusters supported on ceria surfaces
J. Phys. Chem. C 118, 21014 (2014).

16. Changru Ma, Simone Piccinin, and Stefano Fabris
Interface structure and reactivity of water-oxidation Ru-polyoxometalate catalysts on functionalized graphene electrodes
Phys Chem Chem Phys 16, 5333 (2014).

17. Changru Ma, Simone Piccinin, and Stefano Fabris
Rigid- and polarizable-ion potentials for modeling Ru-polyoxometalate catalysts for water oxidation
Acta Chim. Slov. 61, 302 (2014).

18. S Fortuna, P Gargiani, MG Betti, C Mariani, A Calzolari, S Fabris
Structure of self-assembled iron-phthalocyanines on the Au (110) surface through STM imaging and DFT calculations
Microscopie 11 (1), 23-24 (2014)

19. Karolina Kwapien, Simone Piccinin, and Stefano Fabris
Energetics of Water Oxidation Catalyzed by Cobalt Oxide Nanoparticles: Assessing the Accuracy of DFT and DFT+U Approaches Against Coupled Cluster Methods
J. Phys. Chem. Letters. **4**, 4223 (2013)

20. D. Haberer, L. Petaccia, A. V. Fedorov, C. S. Praveen, S. Fabris, S. Piccinin, ... and A. Grueneis
The complete unaltered Eliashberg function of doped graphene from angle-resolved photoemission spectroscopy
Phys. Rev. B **88**, 081401 (2013).

21. P. Ghosh, M. Farnesi Camellone, and S. Fabris
Fluxionality of Au clusters at ceria surfaces during CO oxidation: relationships among reactivity, size, cohesion, and surface defects from DFT simulations
J. Phys. Chem. Letters 4, 2256 (2013).

22. P. Gargiani, G. Rossi, R. Biagi, V. Corradini, M. Pedio, S. Fortuna, A. Calzolari, S. Fabris, J. C. Cezar, N. Brookes, and M. G. Betti
Spin and orbital configuration of Metal Phthalocyanine chains assembled on the Au(110) surface
Phys. Rev. B **87**, 165407 (2013)

23. S. Piccinin, A. Sartorel, G. Aquilanti, A. Goldoni, M. Bonchio, and S. Fabris
Water oxidation surface mechanisms replicated by a totally inorganic tetraruthenium–oxo molecular complex
Proc. Natl. Acad. Sci. **110**, 4917-4922 (2013).

24. L. Szabova, T. Skalab, I. Matolinova, Stefano Fabris, M. Farnesi Camellone, Vladimir Matolin
Copper-ceria interaction: A combined Photoemission and DFT study
Applied Surface Science **267**, 12 (2013).

25. Y. Wang, M. Lingenfelder, S. Fabris, G. Fratesi, R. Ferrando, Th. Classen, K. Kern and Giovanni Costantini
Programming Hierarchical Supramolecular Nanostructures by Molecular Design
J. Phys. Chem. C **117**, 3440 (2013)

26. O. Stetsovych, F. Dvoràk, L. Szabovà, S. Fabris, J. Myslivecek, and V. Matolín
Nanometer-range strain distribution in layered incommensurate systems
Phys. Rev. Letters **109**, 266102 (2012)

27. H. L. Hu, S. Piccinin, A. Laio, and S. Fabris
Atomistic Structure of Cobalt-Phosphate Nanoparticles for Catalytic Water Oxidation
ACS Nano **6**, 10497 (2013)

28. M. G. Betti, P. Gargiani, C. Mariani, R. Biagi, J. Fujii, G. Rossi, A. Resta, S. Fabris, S. Fortuna, X. Torrelles, M. Kumar, M. Pedio
Structural phases of ordered FePc-nanochains self-assembled on Au(110)
Langmuir **28**, 13232 (2012)

29. C. Ma, S. Piccinin, and S. Fabris
Reaction mechanisms of water splitting and H2 evolution by a Ru(II)-pincer complex identified with ab-initio metadynamics in explicit solvent
ACS Catalysis **2**, 1500 (2012)

30. 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)

31. P. Umari and S. Fabris
Importance of semicore states in GW calculations for simulating accurately the photoemission spectra of metal phthalocyanine molecules
J. Chem. Phys. **136**, 174310 (2012)

32. L. Szabova, O. Stetsovych, F. Dvorak, M. Farnesi Camellone, S. Fabris, J. Myslivecek, and V. Matolin
Distinct physico-chemical properties of the first ceria monolayer on Cu(111)
J. Phys. Chem. C **116**, 6677 (2012)

33. S. Fortuna, P. Gargiani, M. G. Betti, C. Mariani, A. Calzolari, S. Modesti, and S. Fabris
Molecule-driven substrate reconstruction in the two-timensional self-organization of Fe-Phthalocyanines in Au(110)
J. Phys. Chem. C **116**, 6251 (2012)

34. T. Sun and S. Fabris
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Nano Letters **12**, 17 (2012)

35. Y. Wang, S. Fabris, Th. W. White, F. Pagliuca, P. Moras, M. Papagno, D. Topwal, P. Sheverdyaeva, C. Carbone, M. Lingenfelder, Th. Classen, K. Kern and G. Costantini
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Chem. Comm. **48**, 534 (2012)

36. S. Fabris, S. Stepanow, N. Lin, P. Gambardella, A. Dmitriev, J. Honolka, S. Baroni, K. Kern
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Nano Letters **11**, 5414 (2011)

37. R. Larciprete, S. Fabris, T. Sun, P. Lacovig, A. Baraldi, and S. Lizzit
Dual path mechanism for the thermal reductioin of graphene oxide
J. Am. Chem. Soc. **133**, 17315 (2011)

38. M. Fanetti, A. Calzolari, ... S. Fabris and A. Goldoni
The Structure and the Molecule-Substrate Interaction in a Co-Octaethyl Porphyrin Monolayer on the Ag(110) Surface
J. Phys. Chem. C **115**, 11560 (2011)

39. S. Piccinin and S. Fabris,
First principles study of water oxidation catalyzed by a tetraruthenium-oxo core within polyoxometalate ligands,
Phys. Chem. Chem. Phys. **13**, 7666 (2011)

40. T. Sun, S. Fabris, and S. Baroni,
Surface precursors and reaction mechanisms for the thermal reduction of graphene oxide,
J. Phys. Chem C **115**, 4730 (2011)

41. L. Szabova, M. Farnesi Camellone, M. Huang, V. Matolin, and S. Fabris
Thermodynamic, electronic and structural properties of Cu/CeO2 surfaces and interfaces from first-principles DFT+U calculations
J. Chem. Phys. **133**, 237455 (2010)

42. 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)

43. 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)

44. 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)

45. 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).

46. 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)

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Nanofaceted Pd-O Sites in Pd-Ce Surface Superstructures Boost Activity in catalytic Combustion of Methane
Angew. Chem. Int. Ed. **48**, 8481 (2009)

48. 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)

49. 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)

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Two-dimensional arrays of Bis(phthalocyaninato)terbium(III) single molecular magnets on Cu (111)
Nano Letters **8**, 3364 (2008).

51. M. Huang and S. Fabris
CO adsorption and oxidation on ceria surfaces from DFT+U calculations
J. Phys. Chem. C **112**, 8643 (2008).

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Looking underneath the fullerenes on Au(110): formation and ordering of surface substrate vacancies
Phys. Rev. B **77**, 153412 (2008)

53. 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)

54. 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)

55. 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).

56. 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)

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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)

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Interaction of Hydrogen with Cerium Oxide Surfaces: a Quantum Mechanical Computational Study
J. Phys. Chem. B 110, 19380 (2006).

59. 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)

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Electron localization determines defect formation on ceria substrates
Science 309, 752 (2005)

61. 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).

62. S. Fabris, S. de Gironcoli, S. Baroni, G. Vicario, and G. Balducci
Reply to comment on "*Taming multiple valency with density functionals: a case study of defective ceria*"
Phys. Rev. B 72, 237102 (2005).

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Electronic and atomistic structures of clean and reduced ceria surfaces
J. Phys. Chem B 109, 22860 (2005)

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Taming multiple valency with density functionals: a case study of defective ceria
Phys. Rev. B 71, 041102 (2005)

65. S. Fabris and Ch. Elsässer
First-principles analysis of intergranular cation segregation to alpha-alumina twin boundaries
Acta Mater. 51, 71-86 (2003)

66. 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)

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A stabilization mechanism of zirconia based on oxygen vacancies only
Acta. Mater. 50, 5171-5178 (2002)

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The Sigma 13 (10-14) twin in alpha-Al2O3: A model for a general grain boundary
Phys. Rev. B 64, 245117 (2001)

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Free energy and molecular dynamics calculations for the cubic-tetragonal phase transition in zirconia
Phys. Rev. B. 63, 94101 (2001)

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Relative energetics and structural properties of zirconia using a self-consistent tight-binding model
Phys. Rev. B 61, 6617 (2000)

Conference proceedings

71. S. Fabris and C. Elsässer
Ab-initio theory of grain-boundary segregation in alumina: atomistics, energetics and electronic structure
MRS Proceedings 751, (2003)

72. S Nufer, A Marinopoulos, S Fabris, C Elsasser, W Kurtz, M Ruhle
Microscopic Analysis of Twin Grain Boundaries in Alumina
Microscopy and Microanalysis 7, 312-313 (2001)

73. N. A. Marks, S. Fabris, and M. W. Finnis,
A coupled compressible and polarizable ionic model applied to oxide crystal structures
Materials Research Society Proceedings 547, 197-202 (1999).

Other publications

74. PhD Thesis
Atomistic modeling of phase transitions in zirconia
Queen's University of Belfast, 2000. Supervisor: Prof. M.W. Finnis

75. Undergraduate Thesis
La stabilità strutturale della zirconia: un'analisi teorica
Università degli Studi di Trieste, 1997. Supervisors: Prof. V. Sergo and Prof. M.W. Finnis

TITOLI

STEFANO FABRIS

Esperienza di ricerca e didattica su tematiche di teoria e metodi di simulazione per la struttura elettronica degli stati condensati

- Didattica: professore a contratto presso la SISSA dal 2010 al 2015 con lezioni su metodi di struttura elettronica numerica per la scienza dei materiali, la scienza delle superfici, e la catalisi eterogenea. (ANNEX I del CV)
- Didattica: lezioni su invito nel programma di workshops e conferenze internazionali su metodi di struttura elettronica numerica per la scienza dei materiali, la scienza delle superfici, e la catalisi eterogenea (ANNEX I e III)
- Ricerca: esperienza di ricerca nel campo della simulazione numerica con metodi di struttura elettronica applicati alla scienza dei materiali, alla scienza delle superfici, e alla catalisi eterogenea. (ANNEX VI)

Titoli dimostranti la congruenza dell'attività scientifica con le discipline ricomprese nel settore concorsuale e in particolare nell'ambito delle simulazioni di struttura elettronica di materiali e processi chimici rilevanti per la catalisi eterogenea e la fotodissociazione dell'acqua

- Si vedano in particolare le pubblicazioni relative agli ultimi 5 anni (ANNEX VI)
- Organizzazione di workshops e conferenze internazionali nelle tematiche oggetto del bando: si vedano I punti I-II dell'ANNEX IV.

Titolo di dottore di ricerca

2000 Ph.D. degree in physics, Queen's University of Belfast, UK;

10/10/2016