

Curriculum Vitae

STEFANO FABRIS



Date of birth: 12 March 1973, Trieste (Italy)
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2018-present Director of the “Istituto Officina dei Materiali” CNR-IOM, Trieste, Italy (www.iom.cnr.it);
2014-2017 Person in charge of the CNR-IOM DEMOCRITOS Theory Unit@SISSA (www.democritos.it);
2005-2013 Head of the theory group@ELETTRA synchrotron facility (www.democritos.it/the-group).

Professional experience

2019-present Research Director, CNR-IOM Theory Unit@SISSA, Trieste, Italy;
2008-2019 Research staff member, CNR-IOM DEMOCRITOS Theory Unit@SISSA, Trieste, Italy;
2004-2008 Tenure-track researcher, DEMOCRITOS Simulation Center, INFN and CNR. *Tenured in 2008*;
2003-2004 Postdoctoral research fellow, INFN-CNR DEMOCRITOS, @SISSA 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.

Scientific production and activity

- 95 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;
- 23000+ citations, H-index 39 (source Google Scholar, October 2020);
- 59 invited talks at international conferences (including 2 ACS meetings, 1 MRS meeting, 1 ECOSS, ..);
- Director/organizer of 12 scientific conferences&workshops (including CECAM, Psi-K).

Awards and distinctions

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);

Teaching

- 2010-2018 *Professore a contratto*, SISSA, Trieste, Italy;
- 2015-2016 *Professore a contratto*, University of Padova, Italy;
- 2010-2011 *Professore a contratto*, University of Trieste, Italy;
- 2006-present Supervisor of 6 PhD, 3 MSc students, 13 postdoctoral fellows;
- 2004-present 16 invited lectures at schools&workshops in the field of computational materials science;
- 2000-2002 Teaching assistant, MSc course, “*Electronic structure of condensed matter*”, University of Stuttgart;
- 1997-1999 Teaching assistant, MSc course, “*Materials science*” Queen's University of Belfast, UK.

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

Principal Investigator, scientist in charge, coordinator

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

Participant:

- FP7-PEOPLE-COST-2011 - CMI 104 *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)

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, Stuttgart, 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) [1182 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) [218]
3. Y. Lykhach, S. M. Kozlov, T. Skala, A. Tovt, V. Stetsovych, N. Tsud, F. Dvorak, V. Johaneck, A. Neitzel, J. Mysliveček, S. Fabris, V. Matolin, K. M. Neyman, J. Libuda
Counting Electrons on Catalyst Nanoparticles
Nature Materials 15, 284–288 (2016) [220]
4. T. Sun and S. Fabris
Mechanisms for oxidative unzipping and cutting of graphene
Nano Letters 12, 17 (2012) [123]
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) [408]
6. M. Farnesi Camellone and S. Fabris
Reaction Mechanisms for the CO Oxidation on Au/CeO₂ catalysts
J. Am. Chem. Soc. 131, 10473 (2009) [266]
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) [218]
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) [359]
9. M. Huang and S. Fabris
CO adsorption and oxidation on ceria surfaces from DFT+U calculations
J. Phys. Chem. C 112, 8643 (2008). [247]
10. QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials
J. Phys. Cond. Matt. 21, 395502 (2009). [16661]

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 André, 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, 2017;
- Luca Dietz, PhD student, Politecnico di Milano, 2014.
- Matteo Ferri, PhD Student, International School for Advanced Studies SISSA, 2018;

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-initio simulation of oxidation processes on graphitic substrates. 6 months visit, August 2011-January 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. **American Chemical Society March Meeting** – San Diego, USA – 25-29/8/2019
2. **American Physical Society March Meeting** – Los Angeles, USA – 5-9/3/2018
3. **17th International Conference on Theoretical Aspects of Catalysis** – Los Angeles, USA 24-28/6/2018
4. **X International Conference Mechanisms of Catalytic Reactions** – Kaliningrad, Russia 2-6/10/2016
5. **College on Multiscale Computational Modeling of Materials for Energy** –International Centre for Theoretical Physics (ICTP), Italy 4-15 July, 2016
6. **Joint MCC-UKCP-EPCC Workshop on Ab initio Periodic Codes** -- STFC Daresbury Laboratory (UK), 19-22/2/2016
7. **American Chemical Society Fall Meeting** – Boston, USA – 16-20/8/2015
8. **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*
9. **National Conference on Condensed Matter Physics - FISMAT 2015** – Palermo, Italy – 28/9-2/10/2015
10. **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*
11. **Energy&Materials Nanotechnology Meeting- EMN 2015** – Istanbul, Turkey–
12. **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*
13. **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*
14. **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*
15. **ICTP Workshop on Advances in Materials Science (KWAMS'13)** – Khartoum – 19-31/1/2013
Title: *Surface-supported Metal Clusters: Insight from Computational Modeling*
16. **UNESCO Advanced Workshop on Solar Energy Conversion** - Bucharest - 21-24/5/2012
Title: *Computational Modeling of New Materials for Solar-driven Fuel Production*
17. **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*
18. **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*
19. **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*
20. **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*
21. **Workshop of the PhD in Nanotechnology** - Università di Trieste, 20-23/9/2011
Title: *Computational Materials Science for Energy Conversion and Storage*
22. **ICTP-TWAS II Latin American Workshop** on Computational Materials Science for Energy and Environmental Applications, Santo André, Brazil - 5-16/9/2011
Title: *Computational modeling of catalytic materials for energy and environmental applications*

23. **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*
24. **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*
25. **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*
26. **Energy Materials Workshop**, Thomas Young Center, London - 7-9/9/2010
Title: *Ab initio modeling of homogeneous catalysts for water oxidation*
27. **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*
28. **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*
29. **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*
30. **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*
31. **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*
32. **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*
33. **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*
34. **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*
35. **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*
36. **Colloquium on "Nanostructured Oxide Surfaces"**, Dipartimento di chimica, Università di Torino, Italy - 23-24/3/2006
Title: *Modeling the surface chemistry of Cerium Oxide using Density Functional Theory*
37. **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*
38. **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*
39. **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*
40. **MMD Matter, Materials, and Devices Meeting**, Genova - 22-25/6/2005
Title: *Taming multiple valency with density functionals: the case of reduced ceria*
41. **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

42. Colloquium at Friedrich-Alexander-Universitaet Erlangen-Nuernberg – 27/1/2016
43. Colloquium at **Technische Universitaet Muenchen** – 9/11/2015
44. Colloquium at **Beijing Computational Science Research Center** (CSRC) – 9/10/2015
45. 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*
46. 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*
47. **Università degli Studi di Brescia** – 16/12/2014 – Host: Prof. Alberto Salvadori
Title: *Computational Modeling of New Materials for Solar-driven fuel production*
48. **University of Tokyo**, Japan – 28/8/2013 – Host: Tsuneyuki
Title: *Computational Modeling of New Materials for Electrochemical Solar-to-Fuel Energy Conversion*
49. **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*
50. **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*
51. 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*
52. **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*
53. 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*
54. **University College Cork**, Ireland - 28/9/11 - Host: M. Nolan
Title: *Catalytic activity of metal clusters and substitutional ions at reducible oxide surfaces*
55. **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*
56. **Molecular Foundry, Lawrence Berkeley National Laboratory**, Berkeley, USA - 28/7/2010 - Host: Jeffrey Neaton
Title: *Catalytic activity of Au nanoclusters supported by Cerium oxide*
57. **Charles University, Prague**, Check Republic - 15/9/2009 - Host: V. Matolin
Title: *Structure and reactivity of metal nanoparticles supported by ceria surfaces*
58. **Tianjin University**, China - 18/09/2009 – Host:
Title: *Reactivity and deactivation of metal nanoparticles supported by reducible oxides: The case of the Au/CeO₂ catalyst*
59. **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*
60. **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.cecama.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.cecama.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);

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, EUROTTECH
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 CMI 104 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 TECHNOLOGY FACILITIES COUNCIL;
PSI - PAUL SCHERRER INSTITUT;
CSIC-CNM - CONSEJO SUPERIOR DE INVESTIGACIONES CIENTIFICAS
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.

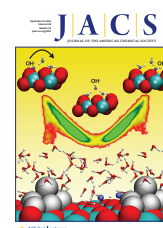
ANNEX VI PUBLICATIONS

17000+ citations, H-index=36 (source Google Scholar, January 2019)

<https://scholar.google.it/citations?user=t7stXLgAAAAJ&hl=it>

International refereed journals

1. Hailiang Zhao, Xia Sheng, Stefano Fabris, Dennis R Salahub, Tao Sun, Lin Du
[Heterogeneous reactions of SO₂ on the hematite\(0001\) surface](#)
The Journal of chemical physics 149 (19), 194703 (2018)
2. Lucie Szabová, Matteo Farnesi Camellone, Fabio Negreiros Ribeiro, Vladimír Matolín, Yoshitaka Tateyama, Stefano Fabris
[Dynamical Solvent Effects on the Charge and Reactivity of Ceria-Supported Pt Nanoclusters](#)
The Journal of Physical Chemistry C 122 (48), 27507-27515 (2018)
3. Nguyen-Dung Tran, Matteo Farnesi Camellone, Stefano Fabris
[Probing the Reactivity of Pt/Ceria Nanocatalysts toward Methanol Oxidation: From Ionic Single-Atom Sites to Metallic Nanoparticles](#)
The Journal of Physical Chemistry C 122 (31), 17917-17927 (2018)
4. P. Giannozzi, et. al.
[QE: Quantum open-Source Package for Research in Electronic Structure, Simulation, and Optimization](#)
Astrophysics Source Code Library (2018)
5. Filip Dvořák, Lucie Szabová, Viktor Johánek, Matteo Farnesi Camellone, Vitalii Stetsovych, Mykhailo Vorokhta, Andrii Tovt, Tomáš Skála, Iva Matolínová, Yoshitaka Tateyama, Josef Mysliveček, Stefano Fabris, Vladimír Matolín
[Bulk hydroxylation and effective water splitting by highly reduced cerium oxide: the role of O vacancy coordinations](#)
ACS Catalysis 8 (5), 4354-4363 (2018)
6. Yaroslava Lykhach, Albert Bruix, Stefano Fabris, Valérie Potin, Iva Matolínová, Vladimír Matolín, Jörg Libuda, Konstantin M Neyman
[Oxide-based nanomaterials for fuel cell catalysis: the interplay between supported single Pt atoms and particles](#)
Catalysis Science & Technology 7 (19), 4315-4345 (2017)
7. Alexander Correa, Matteo Farnesi Camellone, Ana Barragan, Abhishek Kumar, Cinzia Cepek, Maddalena Pedio, Stefano Fabris, Lucia Vitali
[Self-texturizing electronic properties of a 2-dimensional GdAu 2 layer on Au \(111\): the role of out-of-plane atomic displacement](#)
Nanoscale 9 (44), 17342-17348 (2017)
8. 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
9. Matteo Farnesi Camellone, Fabio Negreiros, Lucie Szabová, 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)
10. 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)
11. Y. Lykhach, S. M. Kozlov, T. Skála, A. Tovt, V. Stetsovych, N. Tsud, F. Dvorak, V. Johaneck, A. Neitzel, J. Mysliveček, S. Fabris, V. Matolin, K. M. Neyman, J. Libuda
Counting Electrons on Catalyst Nanoparticles
Nature Materials 15, 284–288 (2016)
12. 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)
13. 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)



14. 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)
15. 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 CeO_x Substrate in Dependence on a Degree of Cerium Oxide Reduction
J. Phys. Chem. C **120**, 2468 (2016)
16. 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)
17. 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).
18. 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).
19. 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).
20. 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).
21. Changru Ma, Stefano Fabris, Alessandro Laio and Simone Piccinin
QMMM: A wrapper for QM/MM simulations with Quantum ESPRESSO and LAMMPS
Computer Physics Communications (2015).
22. 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).
23. 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).
24. 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).
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Structure of self-assembled iron-phthalocyanines on the Au (110) surface through STM imaging and DFT calculations
Microscopie **11** (1), 23-24 (2014)
26. 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)
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Applied Surface Science **267**, 12 (2013).
32. Y. Wang, M. Lingenfelder, S. Fabris, G. Fratesi, R. Ferrando, Th. Classen, K. Kern and Giovanni Costantini
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Atomistic Structure of Cobalt-Phosphate Nanoparticles for Catalytic Water Oxidation
ACS Nano **6**, 10497 (2013)
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Structural phases of ordered FePc-nanochains self-assembled on Au(110)
Langmuir **28**, 13232 (2012)
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38. P. Umari and S. Fabris
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Molecule-driven substrate reconstruction in the two-dimensional self-organization of Fe-Phthalocyanines in Au(110)
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Mechanisms for oxidative unzipping and cutting of graphene
Nano Letters **12**, 17 (2012)
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Chem. Comm. **48**, 534 (2012)
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Oxygen Dissociation by Concerted Action of Di-Iron Centers in Metal-Organic Coordination Networks at Surfaces: Modeling Non-Heme Iron Enzymes
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Dual path mechanism for the thermal reduction of graphene oxide
J. Am. Chem. Soc. **133**, 17315 (2011)
45. 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)
46. S. Piccinin and S. Fabris,

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Phys. Chem. Chem. Phys. **13**, 7666 (2011)
47. T. Sun, S. Fabris, and S. Baroni,
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Thermodynamic, electronic and structural properties of Cu/CeO₂ surfaces and interfaces from first-principles DFT+U calculations
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J. Phys. Chem. C **114**, 13020 (2010)
50. A. Wade, S. Lizzit, L. Petaccia, A. Goldoni, D. Diop, H. Ustunel, S. Fabris, and S. Baroni
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J. Chem. Phys. **132**, 234710 (2010)
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Enhanced Oxygen Buffering by Substitutional and Interstitial Ni point defects in Ceria: A first-principles DFT+U Study
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MRS Proceedings 751, (2003)
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