Curriculum Vitae

STEFANO FABRIS

Date of birth: 12 March 1973, Trieste (Italy)
Address: Istituto Officina dei Materiali – IOM Materials Foundry - Consiglio Nazionale delle Ricerche Area Science Park, Basovizza S.S. 14 Km 163.5, 34149 Trieste, Italy.
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2018-present Director of the "*Istituto Officina dei Materiali"* CNR-IOM, Trieste, Italy (www.iom.cnr.it);
2021-present Italian representative in the *European High Performance Computing Joint Undertaking* EuroHPC (http://eurohpc-ju.europa.eu)
2021-present Italian representative in the European Spallation Source – Instrument Consortium Executive Board
2022-present Member of the Italian group in *Horizon Europe Cluster 4 "Digital, Industry and Space"*
2014-2017 Head of the CNR-IOM 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, Trieste, Italy;
2008-2019 Researcher, CNR-IOM DEMOCRITOS Theory Unit@SISSA, Trieste, Italy;
2004-2008 Tenure-track researcher, DEMOCRITOS Simulation Center, INFM and CNR. *Tenured in 2008*;
2003-2004 Postdoctoral research fellow, INFM-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, UK;
1998 Degree in Materials Science and Engineering, University of Trieste, Italy. 110/100 cum laude.

Scientific production and activity

- ~100 scientific papers published in international journals and refereed conference proceedings: Science, Nature Materials, Nature Comm, Nature Catalysis, PNAS, JACS, PRL, Nano Lett/ACS Nano, Angew Chem Int Ed, …;
- 32000+ citations, H-index 46 (source Google Scholar, January 2023);
- 59 invited talks at international conferences (including 2 ACS meetings, 1 MRS meeting, 1 ECOSS, ..);
- Director/organizer of 13 scientific conferences&workshops (including CECAM, Psi-K, …).

Awards and distinctions

2018 *Abilitazione nazionale* as full professor in physics (sectors 02/B2) & chemistry (03/B1 and 03/A2)
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

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 9 PhD, 4 MSc students, 15 postdoctoral fellows;
- 2004-present 16 invited lectures at schools&workshops in the field of computational materials science;
- 1999-2002 Teaching assistant, MSc course, University of Stuttgart, DE & 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, solar hydrogen, fuel cells; Surface chemistry and heterogeneous catalysis; Defect chemistry of materials; Computational spectroscopy and microscopy.

Main Funding

Principal Investigator, scientist in charge, coordinator

15 M€ PNRR – *Centro Nazionale HPC, Big Data, Quantum Computing – Spoke Materials* 2022-2025

19 M€ MUR L. 205/2017 – *CNR@Elettra2.0* 2021-2026

15 M€ EU-H2020-INFRAIA-2020 - *Nanoscience Foundries and Fine Analysis - Europe|PILOT* 2021-2026

12 M€ EU H2020-INFRAIA-2014/2015 - *Nanoscience foundries and fine analysis for Europe* 2015-2021;

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;

PI and in computational grants: >55 M hours on HPC infrastructures (ISCRA-CINECA, PRACE, …)

Research visits

2015-2016 Technische Universität München (invited *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 the Scientific Committee: HPC4DSR Consortium
- Member of the Advisory Editorial Board for Surface Science – Elsevier Ed
- Associate Editor - Journal of Materials for Renewable and Sustainable Energy - Springer Ed.;
- Member of the Editorial Board for Surfaces – MDPI Ed
- Member of PhD and Master examination committees for: Humboldt University, University of Lyon, Aarhus University; King's College of London; SISSA, University of Ljubljiana; Charles University of Prague; Università Ca' Foscari, Università di Trieste, …;
- 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. *QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials*
   J. Phys. Cond. Matt. 21, 395502 (2009). [22820 citations]
2. 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) [1368 citations]
3. 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) [369]
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) [398]
5. A Chen, X Yu, Y Zhou, S Miao, Y Li, S Kuld, J Sehested, J Liu, T Aoki, S. Fabris et al.
   Structure of the catalytically active copper–ceria interfacial perimeter
   Nature Catalysis 2, 334 (2019) [252]
6. T. Sun and S. Fabris
   Mechanisms for oxidative unzipping and cutting of graphene

Nano Letters 12, 17 (2012) [147]

7. 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) [449]
8. M. Farnesi Camellone and S. Fabris
   Reaction Mechanisms for the CO Oxidation on Au/CeO2 catalysts
   J. Am. Chem. Soc. 131, 10473 (2009) [324]
9. 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) [288]
10. 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) [457]
11. S Piccinin, A Sartorel, G Aquilanti, A Goldoni, M Bonchio, S Fabris
    Water oxidation surface mechanisms replicated by a totally inorganic tetraruthenium–oxo molecular complex
    Proceedings of the National Academy of Sciences **110**, 4917 (2013) [82]
12. *QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials*
    J. Phys. Cond. Matt. 21, 395502 (2009). [22820]

ANNEX I
TEACHING

Graduate and Postgraduate courses

1. ***International School for Advanced Studies – SISSA***. 2010-2018
   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, MSc 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, 2018-2021;
- Xuejun Gong, PhD Student, International School for Advanced Studies SISSA, 2020;
- Mina Taleblou, PhD Student, Università degli Studi di Trieste, 2020;
- Carlo Federico Pauletti, PhD Student, Università degli Studi di Trieste, 2021;

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, 2015-2018
- Joshua Elliott, CNR-IOM, 2018-2020
- Giulia Righi, CNR-IOM, 2019-2021

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. ***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: *Computation al 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 Andrè, 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 chemisrty 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 suppported 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. ***FISMAT-- national conference on condensed matter physics –*** *Scientific Committee*
   30/09-4-10/2019, Catania, ITA
2. ***CECAM workshop -- Interface processes in photochemical water splitting: Theory meets experiment***
   27-30/09/2016, EPFL, Lausanne, CH
3. ***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
4. ***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
5. ***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
6. ***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
7. ***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
8. ***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
9. ***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
10. ***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
11. ***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/
12. ***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/

13. ***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, person in charge, coordinator

PNRR – National Center in High Performance Computing, Big Data and Quantum Computing
Leader of the Spoke Materials and Molecular Sciences,
Other partners involved: CNR Consiglio Nazionale delle Ricerche, SISSA, Università di Milano Bicocca, Università di Trieste, Università di Torino, Politecnico di Torino, Università di Pisa, Università di Firenze, Università di Trento, Università della Calabria, ENEA.
Total funding: 15 M€
Funding of CNR unit: 7.2 M€

Funding period: March 2021- February 2025

MUR L. 205/2017 – CNR@Elettra2.0
Project contractor, Project Leader
Other partners involved: CNR Consiglio Nazionale delle Ricerche,
Total funding: 19 M€

Funding period: 2021- 2027

EU H2020-INFRAIA-2020 - Nanoscience Foundries and Fine Analysis - Europe|PILOT
Project contractor, Member of General assembly for CNR, Co-PI
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, CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE, 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: 15 M€
Funding of CNR unit: 3.2 M€

Funding period: March 2021- February 2025

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: 12 M€
Funding of CNR: 2.4 M€ (of coordinated unit 260 K€)
Funding period: September 2015- March 2021

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

ANNEX VI
PUBLICATIONS

32000+ citations, H-index=46 (source Google Scholar, January 2023)
https://scholar.google.it/citations?user=t7stXLgAAAAJ&hl=it

International refereed journals

1. G Righi, J Plescher, FP Schmidt, RK Campen, S Fabris, A Knop-Gericke, … S Piccinin
On the origin of multihole oxygen evolution in haematite photoanodes
Nature Catalysis 5 (10), 888-899 (2022)
2. M Taleblou, MF Camellone, S Fabris, S Piccinin
Oxidation of Gas-Phase and Supported Pt Nanoclusters: An Ab Initio Investigation
The Journal of Physical Chemistry C 126 (26), 10880-10888 (2022)
3. M Farnesi Camellone, F Dvořák, M Vorokhta, A Tovt, I Khalakhan, … S Fabris, J Mysliveček
Adatom and Nanoparticle Dynamics on Single-Atom Catalyst Substrates
The Journal of Physical Chemistry C 125 (34), 18752-18761(2021)
4. WU Cuixia, SUN Tao, S FABRIS, DU Lin
Ab initio simulations of NO adsorption on hematite (0001) surface: PBE versus PBE+ U
Journal of University of Chinese Academy of Sciences 125 (2022)
5. G Righi, S Fabris, S Piccinin
Oxygen Evolution Reaction on the Fe_3O_4(001) Surface: Theoretical Insights into the Role of Terminal and Bridging Oxygen Atoms
The Journal of Physical Chemistry C 125 (34), 18752-18761(2021)
6. M Ferri, JD Elliott, MF Camellone, S Fabris, S Piccinin
$CuFeO_2$–Water Interface under Illumination: Structural, Electronic, and Catalytic Implications for the Hydrogen Evolution Reaction
ACS Catalysis 11 (4), 1897-1910 (2021)
7. D Knez, G Dražić, SK Chaluvadi, P Orgiani, S Fabris, G Panaccione et al.
Unveiling oxygen vacancy superstructures in reduced anatase thin films
Nano Letters 20 (9), 6444-6451 (2020)
8. M Ferri, J Elliott, S Fabris, S Piccinin
Establishing best practices to model the electronic structure of from first principles
Physical Review B 101 (15), 155201(2020)
9. M Ferri, J Elliott, M Farnesi Camellone, S Fabris, S Piccinin
Ab-initio investigation of a novel photocathode: bulk and surface properties of $CuFeO_2$
The Journal of chemical physics 149 (19), 194703 (2018)
10. JJ Novoa, MF Camellone, S Fabris, RWA Havenith, R Broerb et al.
Two different mechanisms of stabilization of regular p-stacks of radicals in switchable dithiazolyl-based materials1
J. Mater. Chem 100 (8), 5437-5448 (2020)
11. T Francese, S Vela, M Deumal, F Mota, JJ Novoa, MF Camellone, et al.
Two different mechanisms of stabilization of regular π-stacks of radicals in switchable dithiazolyl-based materials
Journal of Materials Chemistry C 8 (16), 5437-5448 (2020)
12. M Ferri, J Elliott, M Farnesi Camellone, S Fabris, S Piccinin
Thermodynamic Stability and Native Point Defects of $CuFeO_2$ Photocathodes in Dry and Electrochemical Environments
The Journal of Physical Chemistry C 123 (49), 29589-29598 (2019)
13. Y Lykhach, S Piccinin, T Skála, M Bertram, N Tsud, O Brummel, et al.
Quantitative analysis of the oxidation state of cobalt oxides by resonant photoemission spectroscopy
The journal of physical chemistry letters 10 (20), 6129-6136 (2019)
14. A Chen, X Yu, Y Zhou, S Miao, Y Li, S Kuld, J Sehested, J Liu, T Aoki, S. Fabris et al.
Structure of the catalytically active copper–ceria interfacial perimeter
Nature Catalysis 2 (4), 334-341(2019)

15. M Farnesi Camellone, A Correa, A Barragán, M Pedio, S Fabris, C Cepek,
Can Atomic Buckling Control a Chemical Reaction? The Case of Dehydrogenation of Phthalocyanine Molecules on $GdAu_2$/Au(111)
The Journal of Physical Chemistry C 123 (11), 6496-6501 (2019)

16. A Tovt, L Bagolini, F Dvořák, ND Tran, M Vorokhta, K Beranová, S. Fabris
Ultimate dispersion of metallic and ionic platinum on ceria
Journal of Materials Chemistry A 7 (21), 13019-13028 (2019)

17. Hailiang Zhao, Xia Sheng, Stefano Fabris, Dennis R Salahub, Tao Sun, Lin Du
Heterogeneous reactions of SO_2 on the hematite(0001) surface
The Journal of chemical physics 149 (19), 194703 (2018)

18. 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)

19. 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)

20. P. Giannozzi, et. al.
QE: Quantum opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization
Astrophysics Source Code Library (2018)

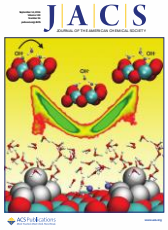
21. Filip Dvořák, Lucie Szabová, Viktor Johánek, Matteo Farnesi Camellone, Vitalii Stetsovych, Mykhailo Vorokhta, Andrii Tovt, Tomáš Skála, Iva Matolínová, Yoshitaka Tateyama, Josef Mysliveček, Stefano Fabris, Vladimír Matolín
Bulk hydroxylation and effective water splitting by highly reduced cerium oxide: the role of O vacancy coordinations
ACS Catalysis 8 (5), 4354-4363 (2018)

22. 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)

23. 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)

24. 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

25. 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)



26. 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)

27. 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
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Nature Materials 15, 284–288 (2016)

28. 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
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Physical Chemistry Chemical Physics 18, 7672 (2016)

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J. Phys. Chem. A, (2016)

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Controlled thermodynamics for tunable electron doping of graphene on Ir(111)
Phys. Rev. B 94, 085427 (2016)

31. K. Ševčíková, L. Szabová, M. Kettner, P. Homola, N. Tsud, Stefano Fabris, V. Matolín
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J. Phys. Chem. C 120, 2468 (2016)

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Temperature effects on the dissociation of hydrogen on ceria surfaces
J. Phys. Chem. C 119, 21567 (2015)

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Adsorption of alkali adatoms on graphene supported by Au/Ni(111)
Physical Review B 92, 075403 (2015).

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Water Oxidation by Ru-Polyoxometalate Catalysts: Overpotential Dependency on the Number and Charge of the Metal Centers
Inorganics 3, 374 (2015).

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Efficient gating of epitaxial boron nitride monolayers by ionic functionalization
Physical Review B 92, 125440 (2015).

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J. Phys. Chem. C 119, 2537 (2015).

37. 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).

38. 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).

39. 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).

40. 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).

41. 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)

42. 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)

43. 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).

44. 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).

45. 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)

46. 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).

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Copper-ceria interaction: A combined Photoemission and DFT study
Applied Surface Science **267**, 12 (2013).

48. 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)

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Nanometer-range strain distribution in layered incommensurate systems
Phys. Rev. Letters **109**, 266102 (2012)

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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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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)

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Formation of hybrid electronic states in FePc chains mediated by the Au(110) surface
J. Phys. Chem. C **116**, 8657 (2012)

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J. Chem. Phys. **136**, 174310 (2012)

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J. Phys. Chem. C **116**, 6677 (2012)

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Molecule-driven substrate reconstruction in the two-timensional self-organization of Fe-Phthalocyanines in Au(110)
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J. Am. Chem. Soc. **133**, 17315 (2011)

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J. Phys. Chem. C **115**, 11560 (2011)

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

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J. Chem. Phys. **133**, 237455 (2010)

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J. Phys. Chem. C **114**, 13020 (2010)

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J. Am. Chem. Soc. **131**, 10473 (2009)

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