Curriculum Vitae

Matteo Farnesi Camellone

- **Date of birth**: 12^{th} January 1976, Padova, Italy
- **Address**: Istituto Officina dei Materiali CNR-IOM-Consiglio Nazionale delle Ricerche c/o Scuola Internazionale Superiore di Studi Avanzati SISSA, Via Bonomea 265, 34136 Trieste, ITALY
- **E-mail**: farnesi@iom.cnr.it

Professional Experience

- **2018-present**: Research (permanent), CNR-IOM DEMOCRITOS Theory Unit@SISSA, Trieste, Italy
- **2013-2018**: Researcher (Fixed Term), CNR-IOM DEMOCRITOS Theory Unit@SISSA, Trieste, Italy
- **2010-2013**: Research Associate, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Bochum, Germany
- **2008-2010**: Postdoctoral Researcher, DEMOCRITOS CNR-IOM c/o SISSA, Trieste, Italy
- **2002-2003**: Compulsory social service at Comune di Padova, Padova, Italy

Education

- **18/06/2008**: Ph.D in Physics at ETHZ (Eidgenössische Technisc he Hochschule Zürich), Zurich, Switzerland
  Supervisor: Prof. Louis Schlapbach
- **11/06/2002**: Degree in Theoretical Physics at University of Padova, Physics Department Galileo Galilei, Padova, Italy
  Supervisor: Prof. Attilio Stella
- **1996**: High School: Liceo Scientifico E. Curiel, Padova, Italy

Scientific Interests

Keywords: Computational materials science, Nanostructured materials for artificial photosynthesis, Hydrogen production/purification and fuel cells, Surface chemistry and heterogeneous catalysis of oxides and oxide-supported metals, Chemical reactions at solid/liquid interfaces, Liquid phase heterogeneous catalysis, Photocatalysis for water oxidation, Structural and dynamical properties of amorphous systems.

Methods

Keywords: Density Functional Theory, Classical Molecular Dynamics, *Ab initio* Molecular Dynamics, *Ab initio* Thermodynamics, Metadynamics, Umbrella Sampling

Computational Skills

- Operating Systems: LINUX, UNIX, WINDOWS. MAC OS X.
- Programming Languages: FORTRAN77, FORTAN90, C/C++, Mathematica.
- Softwares: DL POLY, Moldy, GULP, Quantum-ESPRESSO, CPMD, CP2K, CRYSTAL, GAUSSIAN.

Recent International Projects

- 2013-2016: researcher within the EU FP7-NMP-2012 - "*Design of thin-film nano catalysts for on-chip fuel cell technology*"
- 2012-2013: research member of the Cluster of Excellence RESOLV (EXC 1069), Area C "*Ion Solvation and Charge Transfer at Interface*" (funded by Deutsche Forschungsgemeinschaft)

Computational Grants

- March 2016 -March 2017: PRACE 12^{th} Regular call 2016/2017. Fully granted access of 28 million core hours on the FERMI supercomputer at the CINECA Supercomputing Center for the project "*Modelling proton-coupled electron transfers in water oxidation on hematite*".
- Aug. 2012 - Apr. 2013: PRACE 4^{th} Regular call 2012/2013. Fully granted access of 35 million core hours on the FERMI supercomputer at the CINECA Supercomputing Center for the project "*Towards an atomistic understanding of the selective oxidation of alcohols at the Au/TiO_2(110) solid-liquid interface*".

Teaching Experience

- WS 2012/2013 Teaching assistant in the Course"*Dynamics and Simulation*" held by Prof. Dominik Marx (Master's Program Molecular Sciences [iMOS], in english 30 hours).
  Subjects Covered: Classical and Statistical Mechanics, Quantum Mechanics, Potential Energy Surfaces, Molecular Dynamics.
- WS 2011/2012 Teaching assistant in the Course"*Dynamics and Simulation*" held by Prof. Dominik Marx (Master's Program Molecular Sciences [iMOS], in english 30 hours).
  Subjects Covered: Classical and Statistical Mechanics, Quantum Mechanics, Potential Energy Surfaces, Molecular Dynamics.

Supervision and Training

- 2013-present Lucie Szabova Postdoctoral researcher, Center for Green Research on Energy and Environmental Materials (GREEN), National Institute for Materials Science (NIMS), Tsukuba, Japan (co-supervisor, under the supervision of Dr. Stefano Fabris)
- 2014-2016 Luigi Bagolini Postdoctoral researcher, CNR-IOM c/o SISSA, Trieste, Italy (co-supervisor, under the supervision of Dr. Stefano Fabris)
- 2014-2017 Nguyen-Dung Tran, PhD student, Condensed Matter Theory, SISSA, Trieste, Italy (co-supervisor, under the supervision of Dr. Stefano Fabris)
- 2008-2009 Lucie Szabova, MSc student, Department of Surface and Plasma Science, Charles University of Prague, Prague, Czech Republic (co-supervised, under the supervision of Dr. Stefano Fabris)

Research visits

- 2013 (two weeks): Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Bochum, Germany (*Invited*).
- 2008 (two weeks): Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Bochum, Germany (*Invited*).

Publications

1. M. Farnesi Camellone, J. C. Reiner, U. Sennhauser, and L. Schlapbach
   Efficient generation of realistic model systems of amorphous silica,
   http://arxiv.org/abs/1109.2852
2. M. Farnesi Camellone, J. C. Reiner, U. Sennhauser, and L. Schlapbach
   Formation of electron traps in amorphous silica,
   Phys. Rev. B 76, 125205-6 (2007).
3. M. Farnesi Camellone, T.D. Kühne, and D. Passerone
   Density functional theory study of self-trapped holes in disordered SiO_2,
   Phys. Rev. B 80, 033203-4 (2009).
4. M. Farnesi Camellone and S. Fabris
   Reaction Mechanisms for the CO Oxidation on Au/CeO_2 Catalysts: Activity of Substitutional Au^{3+}/Au^{+} Cations and Deactivation of Supported Au^{+} Adatoms,
   J. Am. Chem. Soc. 131, 10473-10483 (2009).
5. 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, 8481-8484 (2009).
6. P. M. Kowalski, M. Farnesi Camellone, N. N. Nair, B. Meyer, and D. Marx
   Charge Localization Dynamics induced by Oxygen Vacancies On the TiO_2(110) Surface,
   Phys. Rev. Lett. 105, 146405-4 (2010).

7. L. Szabova, M. Farnesi Camellone, M. Huang, V. Matolin, and S. Fabris
Thermodynamic, electronic and structural properties of Cu/CeO_2 surfaces and interfaces from first-principles DFT+U calculation,
J. Chem. Phys. 133, 234705-11 (2010).
8. M. Farnesi Camellone, P. M. Kowalski, and D. Marx
Ideal, defective, and gold-promoted rutile TiO_2(110) surfaces interacting with CO, H_2, and H_2O: Structures, energies, thermodynamics, and dynamics from PBE+U,
Phys. Rev. B 84, 035413-18 (2011).
9. M. Farnesi Camellone and D. Marx
Solvation of Au^+ versus Au^0 in aqueous solution: electronic structure governs solvation shell patterns,
Phys. Chem. Chem. Phys. 14, 937-944 (2012).
10. L. Szabova, O. Stetsovych, F. Dvorak, M. Farnesi Camellone, S. Fabris, J. Myslivecek, and V. Matolin
Distinct Physico-Chemical Properties of the First Ceria Monolayer on Cu(111),
J. Phys. Chem. C 116, 6677-6684 (2012).
11. L. Szabova, T. Skalab, I. Matolinova, S. Fabris, M. Farnesi Camellone, and V. Matolin
Copper-ceria interaction: A combined Photoemission and DFT study,
App. Surf. Sci. 267, 12-16 (2013).
12. M. Farnesi Camellone, and D. Marx
On the Impact of Solvation on a Au/TiO_2 Nanocatalyst in Contact with Water,
J. Phys. Chem. Lett. 4, 514-518 (2013).
13. M. Farnesi Camellone, J. Zhao, L. Jin, Y. Wang, M. Muhler, and D. Marx
Molecular Understanding of Reactivity and Selectivity for Methanol Oxidation at the Au/TiO_2 Interface,
Angew. Chem. Int. Ed. 52, 5780-5784 (2013).
14. 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. Lett. 4, 2256-2263 (2013).
15. M. Farnesi Camellone and D. Marx
Nature and Role of Activated Molecular Oxygen Species at the Gold/Titania Interface in the Selective Oxidation of Alcohols,
J. Phys. Chem. C 118, 20989-21000 (2014).
16. MT Nguyen, M. Farnesi Camellone and R. Gebauer
On the electronic, structural, and thermodynamic properties of Au supported on α-Fe_2O_3 surfaces and their interaction with CO,
J. Chem. Phys. 143, 034704-7 (2015).
17. F. R Negreiros, M. Farnesi Camellone, and S. Fabris
Effects of Thermal Fluctuations on the Hydroxylation and Reduction of Ceria Surfaces by Molecular H_2,
J. Phys. Chem. C 119, 21567-21573 (2015).
18. F. Dvorak**, M. Farnesi Camellone**, A. Tovt, N.-D. Tran, F. R. Negreiros, M. Vorokhta, T. Skala, I. Matolinova, J. Myslivecek, V. Matolin, S. Fabris
Creating single-atom Pt-ceria catalysts by surface step decoration,
Nat. Commun. 7:10801 doi: 10.1038/ncomms10801 (2016).
19. Y. Lykhach, A. Figueroba, M. Farnesi Camellone, A. Neitzel, T. Skala, F. R. Negreiros, M. Vorokhta, N. Tsud, K. C. Prince, S. Fabris, K. M. Neyman, V. Matolin, J. Libuda
Reactivity of Atomically Dispersed Pt^{2+} Species towards H2: Model Pt-CeO_2 Fuel Cell Catalyst,
Phys. Chem. Chem. Phys. 18, 7672 (2016).
20. M. Farnesi Camellone, F. Ribeiro Negreiros, L. Szabova, Y. Tateyama, S. Fabris
Catalytic Proton Dynamics at the Water/solid Interface of Ceria-supported Pt Clusters,
J. Am. Chem. Soc. 138, 11560 (2016).
21. N. Ansari, K. Ulman, M. Farnesi Camellone, N. Seriani, R. Gebauer, S.Piccinin
Hole localization in Fe_2O_3 from density functional theory and wavefunction-based methods,
Phys. Rev. Materials 1, 035404 (2017).
22. A. Correa, M. Farnesi Camellone, A. Barragan, A. Kumar, C. Cepek, M. Pedio , S. Fabris, L. Vitali
Self- texturizing electronic-properties in a 2-dimensional $GdAu_2$ layer on Au(111): the role of out-of-plane atomic displacement,
Nanoscale 9, 17342 (2017).
23. D Munoz-Santiburcio, M. Farnesi Camellone, D. Marx
Solvation-Induced Changes in the Mechanism of Alcohol Oxidation at Gold/Titania Nanocatalysts in the Aqueous Phase versus Gas Phase,
Angew. Chem. Int. Ed. 57, 3327 (2018).
24. F. Dvorak, L. Szabova, V. Johanek, M. Farnesi Camellone, V. Stetsovych, M. Vorokhta, A. Tovt, T. Skala, I. Matolinova, Y. Tateyama, J. Myslivecek, S. Fabris, V. Matolin
Bulk Hydroxylation and Effective Water Splitting by Highly Reduced Cerium Oxide: The Role of O Vacancy Coordination,
ACS Catalysis 8, 4354 (2018).

25. N.-D. Tran, M. Farnesi Camellone, S. Fabris
Probing the Reactivity of Pt/Ceria Nanocatalysts toward Methanol Oxidation: From Ionic Single-Atom Sites to Metallic Nanoparticles,
J. Phys. Chem. C 122, 17917 (2018).
26. L. Szabová, M Farnesi Camellone, F. N. Ribeiro, V. Matolín, Y. Tateyama, S. Fabris
Dynamical Solvent Effects on the Charge and Reactivity of Ceria-Supported Pt Nanoclusters ,
J. Phys. Chem. C 122, 27507 (2018).
27. A. Tovt, L. Bagolini, F. Dvorak, N-D Tran, M. Vorokhta, K. Beranová, V. Johánek, M. Farnesi Camellone, T. Skála, I. Matolínová, J. Myslivecek, S. Fabris, V. Matolín
Ultimate dispersion of metallic and ionic platinum on ceria,
J. Mater. Chem. A, 7, 13019 (2019).
28. M. Farnesi Camellone, A. Correa, A. Barragán, M. Pedio, S. Fabris, C. Cepek, L. Vitali
Can Atomic Buckling Control a Chemical Reaction? The Case of Dehydrogenation of Phthalocyanine Molecules on GdAu2/Au(111),
J. Phys. Chem. C 123, 6496 (2019).
29. A. Chen, X. Yu, Y. Zhou, S. Miao, Y. Li, S. Kuld, J. Sehested, J. Liu, T. Aoki, S. Hong, M. Farnesi Camellone, S. Fabris, J. Ning, C. Jin, C. Yang, A. Nefedov, C. Wöll, Y. Wang, W. Shen
Structure of the catalytically active copper?ceria interfacial perimeter,
Nature Catalysis 2, 334 (2019).
30. Y. Lykhach, S. Piccinin, T. Skala, M. Bertram, N. Tsud, O. Brummel, M. Farnesi Camellone, K. Beranová, A. Neitzel, S. Fabris, K. C Prince, V. Matolín, J. Libuda
Quantitative Analysis of the Oxidation State of Cobalt Oxides by Resonant Photoemission Spectroscopy,
J. Phys. Chem. Lett. 10, 6129 (2019).
31. M. Ferri, J. Elliott, M. Farnesi Camellone, S. Fabris, S. Piccinin
Thermodynamic Stability and Native Point Defects of CuFeO2 Photocathodes in Dry and Electrochemical Environments,
J. Phys. Chem. C 123, 29589 (2019).
32. T. Francese, S. Vela, M. Deumal, F. Mota, J. J Novoa, M. Farnesi Camellone, S. Fabris, R. WA Havenith, R. Broer, J. Ribas-Arino
Two different mechanisms of stabilization of regular π-stacks of radicals in switchable dithiazolyl-based materials,
J. Mater. Chem. C, 8, 5437 (2020) .

** *These authors contributed equally to this work.*

Collaborations

- Prof. Dominik Marx, Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Bochum, Germany (theoretician);
- Dr. Stefano Fabris, CNR-IOM Consiglio Nazionale delle Ricerche, Trieste, Italy (theoretician);
- Dr. Simone Piccinin, CNR-IOM Consiglio Nazionale delle Ricerche, Trieste, Italy (theoretician);
- Dr. Yuemin Wang, Institute of Functional Interfaces, Karlsruher Institut für Technologie, Karlsruher, Germany (experimentalist);
- Prof. Martin Muhler, Lehrstuhl für Technische Chemie, Ruhr-Universität Bochum, Bochum, Germany (experimentalist);
- Prof. Vladimir Matolin, Charles University in Prague, Prague, Czech Republic (experimentalist);
- Dr. Josef Myslivecek, Charles University in Prague, Prague, Czech Republic (experimentalist);
- Dr. Lucia Vitali,Universidad del País Vasco, ES-20018 San Sebastián, Spain (experimentalist);
- Prof. Alessandro Trovarelli, Dipartimento di Scienze e Tecnologie Chimiche, Universita di Udine, Italy (experimentalist);

Conferences and Reports

- 30 June 2004: Quantum Mechanics Calculations of Degradation of Dielectrics in Nanotechnologies, presentation for the project Top Nano 21, EMPA, Dübendorf, Switzerland (talk).
- 8 December 2004: Degradation of Ultrathin Gate Oxides, presentation for the project Top Nano 21, EMPA, Dübendorf, Switzerland (talk).
- September 2005: Generation of Amorphous Silica for Oxides Reliability Investigations, DFT 2005 conference, Geneva, Switzerland (poster presentation).

- February 2006, *Ab initio* Study of Hydrogen States in Amorphous Silica, SPS meeting, Lausanne, Switzerland.
- October 2006, Electron Traps in Amorphous Silica, PhD symposium EMPA, Duebendorf, Switzerland (poster presentation).
- 24 July 2007, Point Defects in Crystalline and Amorphous Silica, SISSA, Trieste, Italy (invited talk).
- 4 October 2007, Point Defects in Crystalline and Amorphous Silica, CEA-Saclay, Paris, France (invited talk).
- 17 September 2009, Reaction Mechanisms for CO Oxidation on Gold Supported CeO_2(111), CNR-INFM SLACS, Cagliari, Italy (invited talk).
- 8 December 2009, Reaction Mechanisms for CO Oxidation on Gold Supported CeO_2(111), Lehrstuhl fuer Theoretische Chemie, Ruhr-Universität Bochum, Bochum, Germany (invited talk).
- 6-10 September 2010, Charge Localization Dynamics induced by Oxygen Vacancies On the TiO_2 Surface, Titania for all seasons: Multifunctionality of an undercover semiconductor, CECAM Workshop, University of Bremen, Germany (poster presentation).
- 18 March 2011: Charge Localization Dynamics induced by Oxygen Vacancies On the TiO_2 Surface, DPG Conference in Dresden, Germany (talk).
- 8-12 October 2012: Charge Localization Dynamics Induced by Oxygen Vacancies on the TiO2(110) Surface and Titania and Gold-promoted Titania Surfaces, CECAM Workshop, University of Bremen, Germany (poster presentation).
- 14-18 October 2013: Computer Simulations of Water/Gold/Titania Interfaces, Functional oxides for emerging technologies, CECAM Workshop, University of Bremen, Germany (poster presentation).
- 7 November 2013: Computer Simulations of Water/Gold/Titania Interfaces, RESOLV C meeting, Bochum, Germany (invited talk).
- 12-14 November 2014: Pt Species at Ceria Surfaces, Reducible oxide chemistry, structure and functions COST Action CM1104, 3^{rd} General Meeting, Barcelona, Spain (talk).
- 8-11 June 2015: Structure and reactivity of the electrode/water interface from *ab-initio* molecular dynamics simulations, chipCAT Workshop Program Low-precious-metal-content catalysts for PEM fuel cells, Dijon, France (talk).

Referee Activity

Journal of Chemical Theory and Computation, Journal of the American Chemical Society, Nature Communications, The journal of Physical Chemistry Letters, Nanoscale, Surface Science, The Journal of Chemical Physics, Physical Chemistry Chemical Physics, The Journal of Physical Chemistry C, Physica Status Solidi (RRL), Solid State Communication, RSC Advances