

Curriculum Vitae
STEFANO FABRIS



Date of birth: 12 March 1973, Trieste (Italy)
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2023-present Director of the Department of Physics and Technologies of Matter – National Research Council;
2023-present Italian representative in the *European XFEL Council* (www.xfel.eu);
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”*
2018-2023 Director of the “*Istituto Officina dei Materiali*” CNR-IOM, Trieste, Italy (www.iom.cnr.it);
2014-2017 Head of the CNR-IOM theory Unit at SISSA – International School for Advanced Studies, Trieste;
2005-2013 Head of the theory group@ELETTRA synchrotron facility.

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, 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, 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, ...;
- 36000+ citations, H-index 46 (source Google Scholar, November 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@Eletra2.0	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, Stuttgart, 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 Ljubljana; 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). [25847 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) [1408 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) [409]
4. 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) [467]
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) [332]
6. T. Sun and S. Fabris
Mechanisms for oxidative unzipping and cutting of graphene
Nano Letters 12, 17 (2012) [155]
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) [466]
8. M. Farnesi Camellone and S. Fabris
Reaction Mechanisms for the CO Oxidation on Au/CeO₂ catalysts
J. Am. Chem. Soc. 131, 10473 (2009) [350]
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) [304]
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) [488]
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) [85]