

# FRANCESCO MERCURI

## PERSONAL DATA

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Email: francesco.mercuri@cnr.it

Current Position: Senior Researcher and Group Leader (permanent position), DAIMON Team, <http://www.daimoners.eu>  
Consiglio Nazionale delle Ricerche (CNR), Istituto per lo Studio dei Materiali Nanostrutturati (ISMN), Bologna, Italy.

Address: Via P. Gobetti 101, 40129 Bologna, Italy.

Nationality: Italian.

Languages: Italian (mother language), English, German, French.

## EDUCATION

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**1998 – 2000** Ph.D. studies in Chemical Sciences, University of Perugia, Italy.

**1997 – 1998** Master in Computational Engineering, University of Perugia (Italy), ISRIM (Italy) and Wessex Institute of Technology (UK).

**1997** Professional Qualification and license to practice the Chemist profession.

**1995 – 1997** Graduation studies in Physics, University of Rome “La Sapienza”, Italy.

**1995** M.Sc. in Chemistry (marks 110/110 cum laude), University of Perugia, Italy.

**1989 – 1997** Graduate studies in Chemistry, University of Perugia, Italy.

## PROFESSIONAL ACTIVITY

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**2002 – 2011** Visiting scientist at: Laboratory for Physical Chemistry of Surfaces at the *École Nationale Supérieure de Chimie de Paris*, France; Institut de Ciència de Materials de Barcelona (ICMAB), *Consejo Superior de Investigaciones Científicas (CSIC)*, Barcelona, Spain; Department of Physical Chemistry and Electrochemistry, *Technische Universität Dresden*, Germany; Inorganic Chemistry Laboratory, Department of Chemistry, *University of Oxford*, UK; Swiss National Supercomputing Centre (CSCS) of the *Swiss Federal Institute of Technologies (ETH)*, Manno, Switzerland.

**2010** Senior Researcher (permanent position), *Consiglio Nazionale delle Ricerche (CNR)* Institute for Nanostructured Materials (ISMN), Italy.

**2005 – 2007** Staff researcher, *Max-Planck-Institut für Chemische Physik fester Stoffe*, Dresden, Germany.

**2001** Researcher (permanent position), *Consiglio Nazionale delle Ricerche (CNR)*, Institute for Nanostructured Materials (ISMN), Bologna, Italy (formerly at the Institute of Molecular Sciences and Technologies, Perugia, Italy).

**1999 – 2000** Research stage at the *Max-Planck-Institut für Festkörperforschung*, Stuttgart, Germany, under the supervision of Prof. M. Parrinello.

## GRANTS AND AWARDS

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- 2000 – 2020** Coordinator and PI of several national and international (FP7, H2020, etc.) research projects on modeling in materials science, multiscale modelling and high-performance computing ("*MOSTOPHOS*", H2020-NMP-2014-two-stage-646259, "*EU-RU.net*", FP7-257511); coordination and supervision of CNR and national research grants; scientific coordination of industrial-academic joint research projects on the development of advance technologies for materials and devices for electronics and optoelectronics.
- 2000 – 2020** Coordinator and PI of several national and international research projects on HPC for materials science (DECI/DEISA, PRACE, CINECA/ISCRA, HPC-Europa, etc.).
- 2006 – 2011** International Research Grants: Short-term mobility, CNR (IT); University of Oxford (UK); HPC-Europa; Germany-Italy bilateral exchanges; Grant "Ville de Paris", Paris (FR); Max-Planck-Society, Dresden (DE).
- 2008** Prize "*Alessandro Vaciago*" for chemistry and physics, Accademia dei Lincei, Italy.

## OTHER ACTIVITIES

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Participation in the scientific/organizing committees of international meetings and workshops on modelling, nanotechnology and materials science (CECAM Workshops, SINFO, materials.it, etc.).

Evaluator for National and International research agencies in fields related to nanotechnology, materials science, computational chemistry and high-performance computing.

Graduate and undergraduate teaching (Computer Sciences, Computational Chemistry, Nanotechnology); supervision of graduation and PhD theses (University of Perugia and University of Bologna, Italy); courses on theoretical and computational chemistry and computational materials science at international schools.

## SCIENTIFIC INTERESTS

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Design, development, implementation, and deployment of simulation strategies on large-scale and HPC infrastructures, artificial intelligence in materials and device simulations, machine learning, deep learning, data-driven technologies.

Technology transfer, research to industry translation, modelling interoperability, research data paradigms and meta-languages.

Multi-scale modeling of materials, processes, and devices for advanced organic and hybrid devices for nanoelectronics and bioelectronics (organic light-emitting and light-harvesting devices, transistors, neuroscience devices).

Advanced computational techniques and modelling of complex systems in chemistry, physics, and materials science for low-dimensional nanosystems, functional surfaces and interfaces, and nanostructured biomaterials.

Multi-scale simulation methods, atomistic modeling, ab-initio techniques, molecular dynamics, coarse-graining, device simulations.

Advanced scientific visualization, 3D graphics and animations, virtual reality, web-based and mobile applications.

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