PAOLO GIANNOZZI – Curriculum Vitæ
(September 2024)

Born 1958 in Poggibonsi (Siena, Italy), Italian citizen, married.

Present Position: Full professor of Condensed-Matter Physics, Department of Mathematics, Computer Science, and Physics, University of Udine
Address: via delle Scienze 206, 33100 Udine, Italy
Phone: +39-0432-558216, e-mail: `paolo.giannozzi@uniud.it`,
web: `https://physicslab.uniud.it/persone/paolo-giannozzi`

Education

- 26 February 1988: Ph.D., University of Lausanne (Switzerland). Thesis: "Magnetic properties of Uranium Dioxide: a theoretical analysis", supervisor Prof. P. Erdös.
- 24 June 1982: Degree in Physics at the University of Pisa (Italy), *cum laude*, under the supervision of Prof. Pastori Parravicini.

Spoken languages: Italian (mother tongue), French, English, some notions of German.

Positions held

- November 2006–September 2024: Professor (associate) at University of Udine. Tenured since November 2009.
- October 1991–October 2006: *ricercatore* (assistant professor) at Scuola Normale Superiore, Pisa, Italy. Tenured since October 1994.
- July 1988–October 1991: Post-Doc at IRRMA (Institut Romand de Recherche Numérique en Physique des Matériaux), Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland.
- June 1983–June 1988: *Assistant Doctorant* at the Institute of Theoretical Physics, University of Lausanne (Switzerland).

I spent several periods as visiting scientist at CECAM in Lausannea (6-7/2011) and Lyon (1-6/1997), Princeton University (9/1999–8/2001), IBM Zurich Laboratories (9-12/1993).

Teaching

- Current: *Modern Physics* for Mathematics, *General Physics I* for Mathematics, *Numerical Methods in Quantum Mechanics* for Physics
- Previously: *General Physics I* for Engineering, *General Physics* for Biotechnology, *Structure of Matter* and *Quantum Mechanics* for Computational Physics.

Since 2006 I supervised 8 diploma works (3 B.Sc. and 2 M.Sc. in Mathematics, 2 M.Sc. in Physics, one M.Sc. in Computational Physics).

Prizes and Honors

- 2013 Fellow of the American Physical Society, Division of Computational Physics.
- 2015 Outstanding Referee, American Physical Society. Member of the Editorial Board of *Electronic Structure*, a new IOP Journal.

Research Interests

I am active in the field of numerical simulations from first principles (Density-Functional Theory and its extensions), applied to various types of materials, in particular: nanostructures, heterostructures, systems of biological interest. I have a specific interest to new computational methodologies and to scientific software for high-performance computing. Specific research topics currently pursued include:

- *Development of scientific software*: I am coordinating the development and porting towards exa-scale (that is: to computers performing 10^{18} operations per second) of Quantum ESPRESSO (`http://www.quantum-espresso.org`): an open-source distribution of software for the calculation of materials properties, based on Density-Functional Theory, plane waves, pseudopotentials. This activity is pursued in the framework of the Horizon-2020 MaX-3 (Materials design at the eXascale) Centre of Excellence (`http://www.max-center.eu`).

- *New methods for simulating electronic transport in nanostructures*: the goal of this activity is to improve the non-equilibrium Green's function method developed by Marco Pala e David Esseni (Polytechnical Department of Engineering an Architecture), by complementing it with electron-phonon interactions coefficients, computed from first principles.

- *Simulation of new biomimetic bidimensional catalysts for rechargeable zinc-air batteries*, PRIN 2DORNOT2D (2022XXJNRS) project, and *Shedding light where 2D materials go 3D: energy transfer and second coordination sphere at biomimetic model surfaces*, PRIN-PNRR (P2022B3WCB) project. The two projects are pursued by two post-doctoral fellows (Asha Yadav and Basant Rhoonde) in collaboration with the experimental group of Erik Vesselli in Trieste. The first project studies the catalytic properties of new heterostructured materials formed by self-assembling layers of flat organometalli molecules (porphyrins) deposited on substrates (e.g., graphene). The second project focuses on Cobalt-cobalamin (vitamin B-12) as a potential catalyzer.

- *Properties and reactivity of deep eutectic solvents (DES)*: PON 2014-2020, Action IV.6 "Green Themes" project, in collaboration with Miguel Angel Soler Bastida, Federico Fogolari, and others. The DES are mixtures characterized by a much lower melting point than that of the separate components. Many DES, in particular NADES (natural DES), are very interesting as potential solvents and reactants with low environmental impact in some important reactions. This study consists in classical molecular dynamics simulations and is pursued in collaboration with experimentalists.

More information can be found in the web site of the *Laboratorio di simulazioni classiche e quantistiche*: `https://physicslab.uniud.it/laboratorio-comp`.

Publications

I am the author of 125 scientific publications in international journals, cited 46000 times in the scientific literature (H-index: 39), data from Web of Science, September 2024.