# PAOLO GIANNOZZI – Curriculum Vitæ (April 2023)

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

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### 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

- Since November 2006: Professor (associate) of Condensed-Matter Physics 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).

# **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.

# 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 or am supervising 7 diploma works (2 B.Sc. and 2 M.Sc. in Mathematics, 2 M.Sc. in Physics, one M.Sc. in Computational Physics).

#### **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 calculations.

Specific research topics currently pursued include:

- Development of scientific software: I am coordinating the development and porting towards exa-scale 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, and pseudopotentials This activity is pursued in collaboration with the Horizon-2020 MaX (Materials design at the eXascale) Centre of Excellence http://www.max-center.eu).
- Properties and reactivity of deep eutectic solvents (DES): PON project 2014-2020, Azione IV.6 "tematiche Green", in collaboration with Miguel Angel Soler Bastida, Federico Fogolari, and others. The DES are characterized by a fusion point that is much lower than for the pure components. They also have an interest as low environmental impact solvents. The initial phase of this activity consists in performing classical molecular dynamics simulations.
- New methods for 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.

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 120 scientific publications in international journals, cited 35000 times in the scientific literature (H-index: 38), data from Web of Science, august 2022.