PAOLO GIANNOZZI – Curriculum Vitæ
(January 2020)

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

Present Position: Professor of Condensed-Matter Physics, Department of Mathematics, Computer Science, and Physics, University of Udine
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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 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 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).

Prizes and Honors

- 2013 Fellow of the American Physical Society, Division of Computational Physics.
- 2015 Outstanding Referee, American Physical Society.

Research Interests

I am active in the field of numerical simulations from first principles (Density-Functional Theory and its extensions), applied to nanostructured materials. I am particularly interested to new computational methodologies and to scientific software for high-performance calculations. This is currently my main line of research, pursued in collaboration with the Horizon-2020 MaX (Materials design at the eXascale) Centre of Excellence (http://www.max-center.eu).

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
- *New methods for transport in nanostructures* and *Transport in interfaces of Ni and Cu on graphene*, in collaboration with the Department of Engineering and Architecture (DPIA) of University of Udine.
- *Structure and electronic properties of Metal-Oxide Framework (MOF)*, in collaboration with Modares University (Iran).
- *Core-level shifts in Mg surfaces exposed to water and oxygen*, in collaboration with IOM-CNR and University of Nova Gorica (Slo).

Conference and School organization (since 2015)

- Introductory School of Renewable Energies, Udine, 14-18 September 2015, 12-17 September 2016, 4-9 September 2017 10-15 September 2018, 2-7 September 2019 (`http://scuola-rinnovabili.`
- ICTP/Psi-k/CECAM School on *Electron-Phonon Physics from First Principles*, ICTP Trieste, 19-23 March 2018
- *FISMAT 2017*, Trieste, 1-5 October 2017
- *Advanced Workshop on High-Performance and High-throughput Materials Simulations using Quantum ESPRESSO*, ICTP, Trieste, 16-27 January 2017
- *Introductory School to Renewable Energy*, Udine, 14-18 September 2015 and 12-17 September 2016
- *Advanced Quantum ESPRESSO Developer Training*, ICTP, Trieste, 19-30 January 2015
- *Quantum Espresso Workshop 2014*, Pennsylvania State University, State College, USA, 16-20 June 2014

Invited talks, schools (since 2015)

- Tutorial omn *Atomistic Simulations for electronic and opto-electronic devices*, SiSPAD, Udine, 3 Settembre 2019
- Summer School on *Particle Physics*, lectures on Relativistic kinematics, Università di Udine, 16 July 2018 and 8-9 July 2019

– *A fresco of contemporary condensed matter physics*, Physics Department, University of Pisa, 27-28 September 2018

– *MaX Hackathon*, Universitat Politècnica de Catalunya, Barcelona, 17-20 July 2018

– Summer School on *Particle Physics*, University of Udine, 16-27 July 2018

– Erice School on *Quantum Crystallography*, Erice, 1-9 Giugno 2018

– Invited talk at mini-workshop *From experiments to theory & models: a computational challenge for Biophysics*, Dipartimento di Fisica, Università di Roma Tor Vergata, 5 December 2017

– CECAM Discussion Meeting on *Quantum Crystallography*, Nancy, 19-20 June 2017

– HPC-TS, SISSA, Trieste, 24-25 February 2016

– Quantum ESPRESSO Spring School, UNC, FCQ, Cordoba (Argentina) 28 September – 2 October 2015

– *Interfacial engineering of P3HT/ZnO hybrid solar cells using phtalocyanines*, invited talk at IPMCM, University of Paris VI, 20 April 2015

– *Supermassive Computations in Theoretical Physics*, Fondazione Bruno Kessler, Povo, Trento, 11 February 2015

– *XIX School of Pure and Applied Biophysics on "Theoretical and Computational Approaches to Biophysics"*, Venice, 26-30 January 2015

Publications

I am the author of more than 100 scientific publications in international journals, cited more than 21000 times in the scientific literature (H-index: 36), data from Web of Science, august 2019. The complete list of my papers can be found on my web page:
`http://www.fisica.uniud.it/~giannozz/articoli.html`.
Here my papers since 2015.

Articles

86. *Improved understanding of metal-graphene contacts*, F. Driussi, S. Venica, A. Gahoi, A. Gambi, P. Giannozzi, S. Kataria, M.C. Lemme, P. Palestri, D. Esseni, Microelectronic Engineering, accepted. DOI: https://doi.org/10.1016/j.mee.2019.111035

85. *Fast hybrid density-functional computations using plane-wave basis sets*, I. Carnimeo, S. Baroni, P. Giannozzi, Electron. Struct. **1**, 015009 (2019), DOI: 10.1088/2516-1075/aaf7d4.

84. *Quantum Crystallography: Current Developments and Future Perspectives*, A. Genoni *et al.*, Chem. Eur. J. **24**, 10881 – 10905 (2018), DOI: 10.1002/chem.201705952.

83. *Advanced capabilities for materials modelling with Quantum ESPRESSO*, P. Giannozzi *et al.*, J. Phys.:Condens. Matter **29**, 465901 (2017). DOI: 10.1088/1361-648X/aa8f79

82. *Reproducibility in density-functional theory calculations of solids*, K. Lejaeghere *et al.*, Science **351** (6280), aad300 (2016). DOI: 10.1126/science.aad3000.

Conference Proceedings and other papers

p31. *Software for quantum simulations of tomorrow*, P. Giannozzi, Il Nuovo Saggiatore **35**, n.5-6, p. 34-38 (2019) https://www.ilnuovosaggiatore.sif.it/article/213

p30. *DFT study of graphene doping due to metal contacts*, P. Khakbaz, F. Driussi, A. Gambi, P. Giannozzi, S. Venica, D. Esseni, A. Gahoi, S. Kataria, M.C. Lemme, Proceedings of the 24th Int. Conference on Simulation of Semiconductor Processes and Devices (SISPAD) 2019, pp.279-282, DOI: 10.1109/SISPAD.2019.8870456

p29. *A Performance Study of Quantum ESPRESSO's PWscf Code on Multi-core and GPU Systems*, J. Romero, E. Phillips, G. Ruetsch, M. Fatica, F. Spiga, and P. Giannozzi, in *Performance Modeling, Benchmarking and Simulation of High Performance Computer Systems*, Proceedings of the 8th International Workshop, PMBS 2017, Denver, CO, USA, November 13, 2017, S. Jarvis, S. Wright, S. Hammond (Eds.), pp. 67-90 (2018) ISBN: 978-3-319-72970-1, DOI: 10.1007/978-3-319-72971-8