Paola Andrea Delcompare Rodríguez

Personal Information

Academic interests:	Condensed Matter Physics. Electronic structure theory and simulation. Density functional theory. First principles molecular dynamics. Photocatalysis. Magneto-electric liquids. Liquid crystals.

Employment

Feb 2023-Current	**Post-doctoral Fellowship** *Istituto Officina dei Materiali (IOM) del Consiglio Nazionale delle Richerche (CNR)*-SISSA. Trieste, Italy. IOM AR 020/2022 TS SISSA, titled: *Modellizzazione multi-scala di liquidi magneto-elettrici basati su derivati degli ossidi di ferro.* funded by the European Union's Horizon 2020 research and innovation program under grant agreement No 899285 (MAGNELIQ: a magneto-electric Liquid To better sensing, https://www.magneliq.eu) Supervisor: Dr. Layla Martin-Samos.
Feb 2022-Jan 2023	**Post-doctoral Fellowship** *Istituto Officina dei Materiali (IOM) del Consiglio Nazionale delle Richerche (CNR)*-SISSA. Trieste, Italy. IOM AR 014/2021 TS SISSA, titled: *Studio da principi primi di processi fotoelettrochimici su interface solido/liquido. Supporto teorico ad utenti del progetto NFFA-Europe Pilot.* Supervisor: Dr. Simone Piccinin.

Academic Background

Nov 2018-March 2022	**Ph.D. in Physics.** *Università degli Studi di Trieste.* Trieste, Italy. Thesis title: A Theoretical study of ultra-thin space charge layers in Hematite photoanodes. Supervisor: Dr. Nicola Seriani.

Sep 2017-Aug 2018 | **Postgraduate Diploma Programme, Condensed Matter Physics.**
International Centre for Theoretical Physics (ICTP) . Trieste, Italy.
Thesis title: An ab initio fully relativistic study of the Ru(0001) surface electronic states.
Supervisor: Dr. Nataša Stojic.
Note: This is a pre-PhD programme with a duration of one year. It includes 12 courses and a research project of 3 months.

Jan 2012-Aug 2017 | **Licenciatura en Física Aplicada**
Escuela de Ciencias Físicas y Matemáticas, Universidad de San Carlos de Guatemala. Guatemala.
Thesis: Computational methods based on quantum entanglement for the analysis of phase transitions in quantum spin-1/2 chains.
Supervisor: Dr. Giovanni Ramírez García.
Note: This is a degree in Applied Physics that includes 10 semesters of courses, an internship and a thesis. The Licenciatura degree is often accepted as a Bachelor degree plus a Master degree in the United States and Europe.

Publications

Jul 2024 | N. Seriani, P. A. Delcompare-Rodriguez, A. K. Adak, D. Pandey, V. Mahamiya, C. Pinilla and H. El-Khozondar. Materials, 2024, 17(14), 3460 (2024).

Sep 2021 | Paola A. Delcompare-Rodriguez, Nicola Seriani. *Ultrathin space charge layer in hematite photoelectrodes: a theoretical investigation.* Journal of Chemical Physics 155, 114701 (2021).

Experience

2019-2021 | **Students mentor.** Postgraduate Diploma Programme. *The Abdus Salam International Centre For Theoretical Physics.* Trieste, Italy.
Coordinator: Mikhail Kiselev.
Resolution of doubts from courses and Mentorship.

Jul 2014-Nov 2014 | **Teaching Assistant.** Classical Mechanics course. *Universidad de San Carlos de Guatemala*, Guatemala.

Awards, Distinctions and Fellowships

Nov 2018 | **PhD Scholarship.** Scholarship financed by the Department of Physics from the University of Trieste with funds from ICTP. *The Abdus Salam International Centre For Theoretical Physics-UNESCO.*

Sep 2017 | **Scholarship in Postgraduate Diploma Programme.** *The Abdus Salam International Centre For Theoretical Physics.* Trieste, Italy.

Sep 2017 | **Magna Cum Laude Award.** *School of Physical Sciences and Mathematics, Universidad de San Carlos de Guatemala.* Guatemala.

Sep 2015	**Erasmus Mundus Stipendium.** *Humboldt-Universität zu Berlin.* Berlin, Germany.
Jul 2014	**Academic Excellence Award.** *Universidad de San Carlos de Guatemala.* Guatemala.

Computational Grants

2022-2023	**ISCRA Type C.** Cineca, Marconi100. *(67,000 CPU hours)*, Unraveling the reaction mechanism of the oxygen evolution reaction at the (110) hematite surface. The grant was obtained as principal investigator.

Seminars/Talks given

Oct 2021	**Research Institute of Physical and Mathematical Sciences.** Invited seminar. *School of Physical Sciences and Mathematics. Universidad de San Carlos de Guatemala.* Guatemala.
Sep 2021	**European Materials Society (E-MRS) fall meeting 2021 (online).** Contributed short talk. "A theoretical study of ultrathin space charge layers in hematite photoelectrodes".
Sep 2021	**Three minutes thesis competition (online).** European Materials Society (E-MRS) fall meeting 2021.
Sep 2021	**VII Student Congress of Physics and Mathematics.** Invited talk.
Jul 2021	**I Guatemalan Physics Congress.** Contributed talk. Guatemalan Physics Association. Guatemala.

Meetings

Apr 2025	**MAGNELIQ: meeting Lubiana** Lubiana, Slovenia
Sep 2024	**MAGNELIQ: meeting Maribor** Maribor, Slovenia
Apr 2024	**MAGNELIQ: meeting Praga** Prag, Cechia
Sep 2023	**MAGNELIQ: M36 meeting Prensilia** Pisa, Italia
Mar 2023	**MAGNELIQ: 5th Project Meeting** Trieste, Italia

Workshops, schools and conferences attended

27/06/2023-29/06/23	**SSBench CECAM Workshop** LAAS-CNRS, Toulouse, France.
16/05/2023-19/05/23	**Workshop on Frontiers in Excited State Electronic Structure Methods: from Spectroscopy to Photochemistry** Trieste, Italy.
09/11/2022-11/11/22	**Advanced Quantum ESPRESSO tutorial: Hubbard and Koopmans functionals from linear response** Trieste, Italy. Attended online.
20/09/2021-23/09/2021	**European Materials Society (E-MRS), Fall meeting 2021.** *Symposium A: Materials for energy applications: hydrogen storage/production, solar cells, super capacitors, thermoelectric and carbon based materials.* Attended online.
24/05/2021-28/05/2021	**Workshop on physics and chemistry of solid/liquid interfaces for energy conversion and storage.** *The Abdus Salam International Centre for Theoretical Physics (ICTP)*. Trieste, Italy. Attended online.
23/02/2021-25/02/2021	**20th International workshop on computational physics and material science: total energy and force methods.** *The Abdus Salam International Centre for Theoretical Physics (ICTP)*. Trieste, Italy. Attended online.
28/09/2020-30/09/2020	**Workshop on excited charge dynamics in semiconductors.** *The Abdus Salam International Centre for Theoretical Physics (ICTP)*. Trieste, Italy. Attended online.
16/04/2020-29/05/2020	**Course of Solid state physics in quarantine.** *The Abdus Salam International Centre for Theoretical Physics (ICTP)*. Trieste, Italy. Attended online.
27/01/2020-31/01/2020	**Computational school on electronic excitations in novel materials using the Yambo code.** *The Abdus Salam International Centre for Theoretical Physics (ICTP)*. Trieste, Italy.
10/06/2019-21/06/2019	**Summer School on classical molecular dynamics for material science, nanotechnology and biophysics.** *International School for Advanced Studies (SISSA)*. Trieste, Italy.
18/03/2019-22/03/2019	**Course of Python.** *The Abdus Salam International Centre for Theoretical Physics (ICTP)*. Trieste, Italy.
09/01/2019-11/01/2019	**19th International workshop on computational physics and material science: total energy and force methods.** *The Abdus Salam International Centre for Theoretical Physics (ICTP)*. Trieste, Italy.

Languages

Spanish:	Mother language.
English:	Advanced (C1).
Italian:	Advanced (C2).
German:	Intermediate-low (A2).
French:	Intermediate-low (A2).

Computational Skills

Programming Languages:	c++, FORTRAN and Python.
First principles software:	Good command of Quantum ESPRESSO, LAMMPS and CP2K.
Others:	Good command of Linux terminal, emacs, LaTeX, Gnuplot, xCrysden, VMD and Mathematica.