Paola Andrea Delcompare Rodríguez

Personal Information

email:	delcompare@iom.cnr.it, pdelcomp@sissa.it, paoladelcompare@gmail.com
Academic interests:	Condensed Matter Physics. Electronic structure theory and simulation. Density functional theory. First principles molecular dynamics. Materials for energy applications. Electrolyte-Semiconductor interface. Water splitting reaction (OER) using Iron oxide as photocatalyst.

Academic Background

Current **Feb 2022- Jan 2023**	**Post-doctoral Fellowship** *Istituto Officina dei Materiali (IOM) del Consiglio Nazionale delle Richerche (CNR)*-SISSA. Trieste, Italy Supervisor: Dr. Simone Piccinin.
Current **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.** *The Abdus Salam 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.

Publications

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).

In progress | **Authors:** Paola A. Delcompare-Rodriguez, Nataša Stojic, Polina M. Sheverdyaeva and Paolo Moras.
Summary: We investigated the spin-orbit effects in the surface electronic structure of Ru(0001). The work was directly motivated by experimental findings of surface state splittings, which were not present in the previous scalar-relativistic studies. We performed the calculations in the plane wave pseudopotential formalism of density-functional theory using a fully-relativistic ultrasoft pseudopotential. We have found that the Ru(0001) surface is characterized by a sizeable spin-orbit splitting of the surface states at the K point at 2.2 eV binding energy. The split surface states have a net magnetization perpendicular to the surface and the in-plane tangential component of the magnetization. The results were discussed in the context of the K-point splittings for noble metals. In addition, our calculations and the latest experiments detected new strong surface states and resonances in Ru(0001).

In progress | **Authors:** Paola A. Delcompare-Rodriguez and Simone Piccinin
Title: Unraveling the reaction mechanism of the oxygen evolution reaction at the (110) hematite surface.
Summary: We aim to determine the reaction mechanism of the oxygen evolution reaction (OER) in the presence of the hematite (110) surface. In order to do it, we computed the free energy difference of every possible reaction step and its respective activation energy. We started from the dehydrogenation of the (110) surface to create holes via 1-site PCET (proton-coupled electron transfer) steps. The goal is to determine the lowest energy sequence of steps that lead to accumulation of holes at the surface, which is a pre-requisite for the multi-hole mechanism seen in experiments. Based on the findings of this first investigation, we examined the possible reaction intermediates that can arise, and use them to determine the next steps. We used a combination of first principles molecular dynamics (FPMD) calculations and thermodynamic integration to sample the system at room temperature. In this way, we expect to have a better approximation of the entropic effects involved in the OER mechanism as well as to determine the effect of the solvent. We performed our calculations using the code cp2k, using the rVV10 exchange and correlation functional in our FPMD simulations. We took into account the localized nature of the d orbitals in the iron atoms in hematite using the DFT + U formalism. This study is a first step more to unravel the possible mechanism of the OER in the (110) hematite and therefore to rationalize the sluggish kinetics of this half reaction in the water splitting reaction.

Experience

2019-2021 | **Students mentor.** Postgraduate Diploma Programme. *The Abdus Salam International Centre For Theoretical Physics.* Trieste, Italy.
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". *Symposium A: Materials for energy applications: hydrogen storage/production, solar cells, super capacitors, thermoelectric and carbon based materials.*
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. "Estudio teórico de las capas de carga espacial ultradelgadas en fotoelectrodos de hematita". Guatemala.
Jul 2021	**I Guatemalan Physics Congress.** Contributed talk. Guatemalan Physics Association. Guatemala.

Workshops, schools and conferences attended

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:	Intermediate-high (B2).
German:	Intermediate-low (B1).
French:	Intermediate-low (A2).

Computational Skills

Programming Languages:	c++, FORTRAN and Python.
Electronic structure calculations software:	Good command of Quantum ESPRESSO and CP2K. Knowledgeable in Yambo.
Others:	Good command of Linux terminal, emacs, Gnuplot, VMD and Mathematica.
Text processing:	LaTeX.