

Curriculum Vitae - Roberta POLONI

Place and date of birth: Macerata (Italy), March 4th, 1979

Education and Work Experience

10/2024: CNRS Researcher (DR2) at SIMaP in Grenoble;

02/2022: Habilitation à diriger des recherches;

10/2014: CNRS Researcher (CR) at SIMaP;

2010-2013: Postdoc at the University of California, Berkeley and the Molecular Foundry (LBNL), US;

2007-2009: Postdoc at the ICMAE (Institut de Ciència de Materials de Barcelona), Spain;

2004-2007: PhD in Condensed Matter Physics from the Université Lyon 1 at ESRF, France;

2000-2004: Laurea in Physics *cum laude*, Università di Camerino, Italy.

Supervision, Management, and Animation of Research

- 2022 - present: External member of the Conseil de Faculté des Sciences de Lyon;
- 2021 - 2023: Member of bureau of GDR Rest;
- 2023: organization of school *Introductory school of quantum computing for physicists and chemists*, Grenoble;
- 2023: Animation of a discussion group *Nouveaux enjeux pour les méthodes numériques - IA* within the initiative of the Institute of Physics at CNRS together with Magali Benoit and Nicola Vigano;
- 2024: Organizer of the 27th ETSF conference *European Theoretical Spectroscopy Facility*, Marseille;
- 2025: Organizer of the symposium *Advanced interoperability in atomistic simulations of materials* at E-MRS Fall 2025, Warsaw;
- 2025: Member of the Comité d'évaluation of ANR for CE29 *Chimie analytique, chimie théorique et modélisation*;
- 2018-present: main proposer of 7 grants (ANR, MIAI, ILL PhD fundings, IMEP2, Emergence, etc.);
- 2017-present: supervision of 9 PhD students (4 ongoing) and 6 postdocs (2 ongoing).

Collective Responsibilities

- 2024-present: member of Bureau Committee for Integration and Diversity at SIMaP;
- 2022-present: representative at SIMaP - Conseil de laboratoire as *membre nommé*;
- 2021-2022: leader of a working group to create a shared computing infrastructure at SIMaP;
- 2020-present: member of the CT9 (comité expertise thématique 9: Physics, chemistry and materials properties) Committee of GENCI;
- 2019-present: web Master of the group at SIMaP;
- 2019-2021: co-organizer of Lab seminars;
- 2018-present: member of 12 PhD juries.

Communication Activities

2017 : invited talk at *The conference on gender, career paths and networking*, Berlin (Germany);

2019 : invited talk on Women in Science at the ILL PhD students group meeting, Grenoble;

2020 : invited talk on carbon capture technologie at the Faculty of Langues Etrangères at Grenoble (20 students);

2021, 2022 : invited talk at high school in occasion of the celebration of 11-F Women in Science (120 students, Cáceres, Spain) 2h talk about science and career plus discussion;

2022, 2023 : Fête de la Science at SIMaP.

Bibliometry

50 publications in peer-review journals;

h-index: 25;

Citations: around 3400 from Google Scholar

Invited schools, seminars, and conferences (since 2022)

2025 Reunión Bienal de la Real Sociedad Española de Química, Bilbao (Spain);

2025 Workshop: The determination of Hubbard parameters: progress, pitfalls, and prospects, Gandia (Spain);

2025 Totemic School: Tools for Energy Materials Modelling Acceleration, Corsica;

2024 CECAM Workshop on *Machine Learning Interatomic Potentials and accessible Databases*, Grenoble, (*Artificial-neural-network based exchange and correlation functional for transition metal complexes*);

2024 AI, Chemistry, and Reactivity Workshop - Département de Chimie Moléculaire - DCM Grenoble, *Artificial-Neutral Network-based Exchange and Correlation Functional in DFT*;

2024 IAMAT Plenary meeting, Toulouse (France), (*Machine learning for DFT functionals*);

2024 MOF2024, Singapore, 9th International Conference on Metal-Organic Frameworks Open Framework Compounds, *Engineering the electronic structure properties of metal-organic frameworks using advanced ab initio methods: from photoresponsive to spin-crossover materials*;

2024 MOFSIM24, Montpellier (France), *Insights into the electronic structure properties of MOFs by advanced ab initio methods*;

2023 International of Conference of Women in Exascale, Berlin (Germany), *Insight into the electronic structure properties of MOFs via many-body perturbation theory*;

2023 GDR Rest annual meeting, Oleron (France), *Engineering the electronic structure properties of metal-organic frameworks using ab initio methods: from photoresponsive to spin-crossover materials*;

2023 Trinity College, Dublin (Ireland), invited seminar by Prof. Alessandro Lunghi, *Ab initio calculations of spin splitting energies in transition metal complexes: from molecules to metal-organic frameworks*;

2023 School in Machine Learning in Roscoff, (France), 3h lecture + tutorial invited by GDR IAMAT;

2022 International Workshop on Porous Magnetic Materials, Paris, *Spin crossover MOFs for gas related applications*;

2022 Webinar GDR Rest, monthly seminars, *Spin state energetics in Fe complexes: novel advancements*;

2022 Grenoble (France), Lab seminar series at LiPhy, *Photoswitching metal-organic frameworks for efficient gas capture and release applications*;

2022 Grenoble (France), CpiC-12 Conference, Plenary Speaker, *Photoswitching metal-organic frameworks*.