Stefano **Racioppi**, Ph.D.

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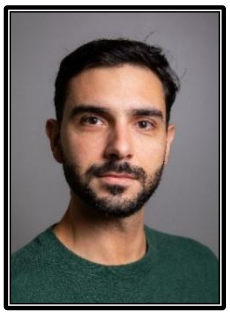

Professional Experience

09/2025 – present Research Associate, *University of Cambridge*, UK.
Group: Prof. Chris Pickard.

03/2021 – 08/2025 Postdoctoral researcher, *State University of New York at Buffalo*, USA.
Group: Prof. Eva Zurek.

07/2023 – 09/2023 Visitor, *Aalto University*, Finland.
Group: Prof. Patrick Rinke.

02/2019 – 02/2021 Postdoctoral researcher, *Chalmers University of Technology*, Sweden.
Group: Prof. Martin Rahm.

Education

10/2015 – 01/2019 Ph.D. in Industrial Chemistry, *University of Milan*, Italy. Supervisors: Prof. Angelo Sironi; Prof. Piero Macchi; Prof. Pierluigi Mercandelli.

11/2018 – 01/2019 Scholarship recipient, National Interuniversity Consortium of Materials Science and Technology (INSTM), *University of Milan*, Italy. Supervisor: Prof. Angelo Sironi.

10/2016 – 03/2018 Visiting student at the *University of Bern*, Switzerland. Host: Prof. Piero Macchi.

10/2013 – 10/2015 Master's degree in Industrial Chemistry, *University of Padua*, Italy. Supervisors: Prof. Armando Gennaro; Prof. Laura Orian. Final grade: 110/110

10/2010 – 09/2013 Bachelor's degree in Industrial Chemistry, *University of Padua*, Italy. Supervisor: Prof. Armando Gennaro.

Research Interests

- Computational and Theoretical Chemistry.
- Quantum Crystallography and Crystal Structure Prediction.
- High Pressure Chemistry.
- Chemical Bonding.
- Material and Planetary Science.
- Superconductivity.
- Catalysis.

Distinctions

03/2025 Marie Skłodowska-Curie Actions (MSCA) Postdoctoral Fellowship, Seal of Excellence 2025.

09/2019 Best Ph.D. Thesis Award by the Italian Crystallographic Association (AIC).

07/2017 Outstanding poster prize offered by Wiley – Journal of Computational Chemistry and International Journal of Quantum Chemistry. Workshop on ab Initio Modeling in Solid State Chemistry with CRYSTAL, *Minneapolis*, USA.

Memberships

2025 – present Trinity Hall College of Cambridge

2024 – present European Crystallographic Association (ECA).

2021 – present American Physical Society (APS).

2018 – present Italian Crystallographic Association (AIC).

2018 – 2019 Swiss Society for Crystallographic (SGK/SSCr).

External Fundings, Proposals and Scholarships

05/2025 Awarded: Proposal experiment, *Structural Determination of Al_2O_3 at super-Earth Conditions – AlO Discovery,* Omega Laser Facility at the Laboratory for Laser Energetics (LLE); 1 shot day awarded. PI: Dr. Racioppi S.

04/2025 Awarded: Beamtime at the European Synchrotron Radiation Facility (ESRF); *Diagnosing Electride Formation in Ca up to 40 GPa with XANES and SCXRD;* 18 shifts awarded. PI: Dr. Chin, D. A.; co-PI: Dr. Racioppi, S.

04/2024 Awarded: 34th European Crystallographic Meeting Scholarship; € 300.

09/2023 – 08/2026 Contributed to the proposal's writing: *High Energy Density Quantum Matter - Renewal*; Award number: LOI-0000043230; Source of Support: Department of Energy (DOE); PI: Dr. Collins G.W.; Co-PIs: Dr. Deemyad S.; Dr. Hemley R. J.; Dr. Zurek E.; $ 2,100,000.

02/2023 Awarded: Beamtime at Laser-lab Europe LENS; *Tuning Electrical Conductivity of Aurophilic Interactions by Compression* (ID: 22396); PIs: Dr. Racioppi S., Dr. Poreba T.; Prof. Macchi P.

09/2022 Awarded: Seed Funding Project; Center for Matter at Atomic Pressure (CMAP); $ 3500.

10/2018 – 01/2019 Awarded: Scholarship; National Interuniversity Consortium of Materials Science and Technology (INSTM); PI: Prof. Sironi A.; € 5862.

05/2018 Awarded: Travelling Grant; Ettore Majorana Foundation; € 600.

Publications

Total number of publications: 24 (16 as first author, 6 as corresponding author (*)).
Total number of citations: 244.
H-index: 10.

(28.) Liu, Z.; **Racioppi, S**.; Hilleke, K. P.; Pandit, A.; Ma, S.; Hermann, A.; Yan, D.; Zurek, E.; Miao, M. Non-local Chemistry Driven by Cation-Anion Size Disparity in Helium Inserted Compounds under High Pressure, *arXiv:2511.23400*.

(27.) Farraj, H.; **Racioppi, S.**; Garbarino, G.; Ahart, M.; Mondal, A.; Parra, S. G.; Smith, J. S.; Cohen, R. E.; Zurek, E.; Cabana, J.; Hemley, R. Novel Pressure-Induced Transformations of $PbTiO_3$, *arXiv:2511.05756*.

(26.) **Racioppi, S.***; Zurek, E. Quantum Effects or Theoretical Artifacts? A Computational Reanalysis of Hydrogen at High-Pressure, *arXiv:2510.02098.*

(25.) Ocampo, I. K.; Kim, D.; Smith, R. F.; Coppari, F.; **Racioppi, S.**; Zurek, E.; Rygg, J. R.; Chin, D. A.; Millot, M.; Eggert, J. H.; Duffy, T. S.; Atomic-level structure and pressure-density response of Fe-O compounds at deep Earth and exoplanetary interior conditions, *under review* in *Physics of the Earth and Planetary Interiors*.

24. Coleman, A. L.; Singh, S.; Lockard, T.; Ocampo, I. K. Lazicki, A. E.; Gorman, M. G.; **Racioppi, S.**; Krygier, A. G.; Wehrenberg, C. E.; Ahmad, R.; Hamel, S.; Han, S.; Ginnane, M. K.; Swift, D. C.; Bonev, S. A.; Zurek, E.; Duffy, T. S.; Eggert, J. H.; McNaney, J.; Smith, R. F. Body-centered cubic phase transformation in gold at TPa pressures. *PRL*, **2025**.

23. **Racioppi, S.***; Zurek, E. Using Topology to Predict Electrides in the Solid, *J. Phys. Chem. A*, **2025**.

22. **Racioppi, S.***; Zurek, E. Activation of Semicore Electrons in Alkali Metals and Their Role in the B1–B2 Phase Transition under Pressure, *J. Am. Chem. Soc*, **2025**, *147*, 36, 32745-32751.

21. Storm, C. V.; **Racioppi, S.**; Duff, M. J.; McHardy, J. D.; Zurek E.; McMahon, M. I. Experimental Evidence of Interstitial Electron Density in Transparent Dense Sodium, *Commun. Mater*, **2025**, *6*, 201.

20. **Racioppi, S.**; Zurek, E. High-Pressure Electrides: A Quantum Chemical Perspective, *Annu. Rev. Mater. Res.*, **2025**, *55*, 421-442.

19. **Racioppi, S.**; Saffarin-Deemyad, I.; Holle, W.; Belli, F.; Ferry, R.; Kenney-Benson, C.; Smith, C. J., Zurek, E.; Deemyad, S. Phase Lithium's low-temperature phase transitions: Insights into quantum lattice dynamics and superconductivity, *PRB*, **2025**, *111*, 054111.

18. **Racioppi, S.**; Zurek, E. Looking at High-Pressure Electrides Through the Lens of Quantum Crystallography: The Case of Simple Cubic Calcium, *Acta Cryst.*, **2025**, B81.

17. **Racioppi, S.**; De la Roza, A.; Hajinazar, S.; Zurek, E. Powder X-Ray Diffraction Assisted Evolutionary Algorithm for Crystal Structure Prediction, *Digit. Discov.*, **2025**, 4, 73-83.

16. **Racioppi, S.**; De la Roza, A.; Hajinazar, S.; Zurek, E. PXRD-Assisted Crystal Structure Predictions, *Acta Cryst.*, **2024**, A80, e396.

15. **Racioppi, S.**; P.; Hyldgaard, P.; Rahm, M. Quantifying Atomic Volume, Partial Charge and Electronegativity in Condensed Phases, *J. Phys. Chem. C*, **2024**, 128, 4009-4017.

14. **Racioppi, S.***; Storm, C. V.; McMahon, M. I.; Zurek, E. On the Electride Nature of Na-hP4, *Angew. Chem. Int. Ed.* **2023**, e202310802.

13. **Racioppi, S.**; Miao, M.; Zurek, E. Intercalating Helium into A-site Vacant Perovskites, *Chem. Mater.* **2023**, 35, 4297-4310.

12. Fang, M.; Srikanth Kumar, G.; **Racioppi, S.**; Zhang, H.; Zurek, E.; Lin, Q. Hydrazonyl Sultones as Stable Tautomers of Highly Reactive Nitrile Imines for Fast Bioorthogonal Ligation Reaction, *J. Am. Chem. Soc.* **2023**, 145, 18, 9959-9964.

11. **Racioppi, S.**; Lolur, P.; Hyldgaard, P.; Rahm, M. A Density Functional Theory for the Average Electron Energy, *J. Chem. Theory Comput.* **2023**, 19, 799-807.

10. Antle, J.; Kimura, M.; **Racioppi, S.**; Lang, M.; Damon, C.; Gatley-Montross, C.; Sánchez B., L.; Miller, D.; Zurek, E.; Brown, A.; Gast, K.; Simpson, S. Applying Density Functional Theory to Common Organic Mechanisms: A Computational Exercise, *J. Chem. Educ.* **2023**, 100, 355-360.

9. **Racioppi, S.**; Orian, L.; Gennaro, A.; Isse, A. Solvent Coordination Effect on Copper-Based Molecular Catalysts for Controlled Radical Polymerization, *Catalysts* **2022**, 12, 1656.
8. Poręba, T.; **Racioppi, S.***; Garbarino, G.; Morgenroth, W.; Mezouar, M. Investigating the Structural Symmetrization of CsI_3 at High Pressures through Combined X-ray Diffraction Experiments and Theoretical Analysis, *Inorg. Chem.* **2022**, 61, 10977-10985.
7. Della Pergola, R.; Garlaschelli, L.; Macchi, P.; Ruffo, R.; **Racioppi, S.**; Sironi, A. From Small Metal Clusters to Molecular Nanoarchitectures with Core-Shell Structure: Synthesis, Redox Fingerprint, Theoretical Analysis and Solid-State Structure of $[Co_{38}As_{12}(CO)_{50}]^{4-}$, *Inorg. Chem.* **2022**, 61, 9888-9896.
6. Kumar, G. S.; **Racioppi, S.**; Zurek, E.; Lin, Q. Superfast Tetrazole−BCN Cycloaddition Reaction for Bioorthogonal Protein Labeling on Live Cells, *J. Am. Chem. Soc.* **2022**, 144, 57–62.
5. **Racioppi, S.**; Rahm M. In-Situ Electronegativity and the Bridging of Chemical Bonding Concepts, *Chem. Eur. J.* **2021**, 27, 18156-18167.
4. **Racioppi, S.***; Sironi, A.; Macchi, P. On Generalized Partition Methods for Interaction Energies, *Phys. Chem. Chem. Phys.* **2020**, 24291-24298.
3. **Racioppi, S.**; Andrzejewski, M.; Colombo, V.; Sironi, A.; Macchi, P. Different Metallophilic Attitudes Revealed by Compression, *Inorg. Chem.* **2020**, 59, 2223−2227.
2. **Racioppi, S.***; Della Pergola, R.; Colombo V.; Sironi, A.; Macchi, P. Electron Density Analysis of Metal Clusters with Semi-Interstitial Main Group Atoms. Chemical Bonding in $[Co_6X(CO)_{16}]^-$ Species, *J. Phys. Chem. A* **2018**, 122, 5004-5015.
1. Della Pergola, R.; Sironi, A.; Colombo, V.; Garlaschelli, L.; **Racioppi, S.**; Sironi, A.; Macchi, P. Periodical trends in $[Co_6E(CO)_{16}]^-$ clusters: Structural, synthetic and energy changes produced by substitution of P with As, *J. Organomet. Chem.* **2017**, 849-850, 130-136.

Invited and Contributed Talks and Seminars

Talks

06/2025 24th Biennial International Conference on the Science of Compression in Condensed Matter (SCCM): Computational Methods: Theory, Codes and Applications (FMDA/B).

06/2025 Crystal Structure Prediction Workshop, a Practical Approach, Poitiers.

09/2024 4th European Symposium on Chemical Bonding (CBOND2024).

08/2024 34th European Crystallographic Meeting (ECM34); Microsymposium M27: High Pressure Crystallography: Exploring Structure and Method Development at Extreme Conditions.

07/2024 Gordon Research Seminar (GRS), Research at High Pressure.*

07/2023 28th AIRAPT and 60th EHPRG International Conference on High Pressure Science and Technology; Session: Chemical Bonding.

03/2022 American Physical Society (APS) March Meeting; Session G24: Matter at Extreme Conditions: Phase Transitions.

09/2021 Italian Crystallographic Association (AIC) XLIX Meeting.*

06/2018 International School of Crystallography in Erice; 52nd Course: Quantum Crystallography.

Seminars

11/2025 Chicago/DOE Alliance Center (CDA) Virtual Seminar Series; *Host*: Prof. Russell Hemley.*

05/2025 Cambridge Crystallographic Data Centre (CCDC), Virtual Seminar; *Host*: Dr. Fabio Montisci.*

07/2024 High Energy Density Science Center (HEDS) Virtual Seminar Series; Lawrence Livermore National Laboratory (LLNL, USA); *Host*: Dr. Federica Coppari.*

01/2024 *University of Milan* (Italy), Dep. of Chemistry; *Host*: Prof. Davide Proserpio.*

08/2023 *Aalto University* (Finland), Dep. of Physics; *Host*: Prof. Patrick Rinke.*

06/2023 *University of Oviedo* (Spain), Dep. of Chemistry; *Host*: Prof. José Manuel Recio.*

04/2023 Italian Young Crystallographers (GCI) *Happy Hour* Virtual Seminar; *Host*: Dr. Marta Morana.*

03/2022 Chicago/DOE Alliance Center (CDA) Virtual Seminar Series; *Host*: Prof. Russell Hemley.*

* = invited

Conference and Workshop Appointments

07/2026 Elected chair of the Gordon Research Seminar (GRS), Research at High Pressure.

07/2025 Co-organizer of the "*High Energy Density Physics: Quantum Materials and Quantum Phenomena*" session at the 24th Biennial Conference on Science of Compression in Condensed Matter (SCCM).

06/2025 Co-organizer of a workshop on the crystal structure prediction code XtalOpt (co-organizer: Prof. Eva Zurek) at the Crystal Structure Prediction Workshop, a Practical Approach, held in Poitiers, France.

05/2025 Moderator at the *Graduate Student Symposium* (GSS) at SUNY Buffalo.

06/2022 Co-organizer of a workshop on the crystal structure prediction code XtalOpt (co-organizer: Prof. Eva Zurek) at the International School of Crystallography in Erice; 56th Course: Crystallography under extreme conditions.

06/2022 Co-organizer of a workshop on computational chemistry techniques (co-organizer: Dr. Julia Contreras-García) at the International School of Crystallography in Erice; 56th Course: Crystallography under extreme conditions.

Teaching and Supervision

2025 Demonstrator for a course in the Scientific Computing MPhil on Electronic Structure and Density Functional Theory.

2021/2025 Co-supervisor of three PhD students (Morgan Reddington, Masashi Kimura, Isaac Ampersand-Kwadwo Akwetey) and supervisor of two undergraduate students (Amelia Kelly, Jarrod DuMond).

01/2024 Special virtual lecture for the students of the general chemistry course at *the University of Milan* – Host: Prof. Davide Proserpio. "*History and Evolution of the Electronegativity*"

2022 – 2023 Hosted online workshops for the usage of the crystal structure prediction code XtalOpt.

2021 Supervisor of a high school student (Henry Feng) for summer project.

2017 – 2019 Co-supervisor of two master students (Stephanie Terruzzi and Simona Sorbara).

2018 – 2019 Teaching assistant, physical chemistry II, 2nd year degree in Industrial Chemistry.

2015 – 2016 Teaching assistant, general and inorganic chemistry, 3rd year degree in Physics.

Computational Developments

Electronegativity in gas-phase: https://github.com/SteRacioppi/Chi-bar-Atomic-and-Molecular-Electronegativity
Electronegativity in solid: https://www.scm.com/doc/BAND/Expert_Options/Restarts.html

Public Service and Outreach

2025 Interviewed by *News Center - News & information from UB*, ***Core electron bonding may not always require extreme pressure, study finds***, regarding our paper "*Activation of Semicore Electrons in Alkali Metals and Their Role in the B1-B2 Phase Transition under Pressure*" published in *JACS*.

2025 Interviewed by *Science News*, ***A new iron compound hints 'primordial' helium hides in Earth's core***, regarding the discovery of helium bearing iron at high pressure.

2023 Interviewed by *News Center - News & information from UB*, ***Sodium's high-pressure transformation can tell us about the interiors of stars, planets***, regarding our paper "*On the Electride Nature of Na-hP4*" published in *Angewandte Chemie*.