Alessandro Caruso

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Employment

Postdoctoral Researcher | AG Clementi **2023–present**
Freie Universität Berlin *Berlin (BE), Deutschland*

- **Project 1**: I have designed and implemented in PyTorch a self-attention framework, namely RANGE, that uses virtual nodes to achieve long-range message-passing in invariant and equivariant graph neural networks (1 manuscript).
- **Project 2**: I am currently working on including nuclear quantum effects in coarse-grained biomolecular simulations using message-passing neural networks (SchNet, PaiNN) with long-range corrections to model the collective spring forces in path-integral molecular dynamics (in progress).

Graduate Student Researcher | Paesani Research Group **2018–2023**
University of California, San Diego *La Jolla (CA), USA*

Development of many-body interaction potentials for the description of ions and small molecules in water.

- **Project 1**: I designed and implemented with scikit-learn an active learning framework for constructing molecular training sets, aiming to minimize the number of labels required during the training of atomistic potentials (1 manuscript).
- **Project 2**: I developed halide-water many-body force fields using permutationally invariant polynomials (in-house C++ implementation), collected the DFT and coupled-cluster reference data, and determined the structural and spectroscopic (EXAFS) properties of gas-phase clusters and bulk phase via MD and PIMD simulations (LAMMPS, enhanced sampling with PLUMED) (2 manuscripts).
- **Project 3**: I developed deep neural network potentials of water (using DeePMD-kit), trained on bulk data I generated from MD simulations, to study its structure from boiling to the supercooled regime (2 manuscripts).
- **Project 4**: I performed DFT reference calculations and trained molecular force fields to assess the accuracy of density-corrected functionals in the description of ion-water interactions (1 manuscript).

Graduate Teaching Assistant **2018–2023**
University of California, San Diego *La Jolla (CA), USA*

Education

Ph.D. in Theoretical and Computational Chemistry **2018–2023**
University of California, San Diego *La Jolla (CA), USA*
Supervisor: F. Paesani

MSc in Physical Chemistry **2016–2018**
Università degli Studi di Roma "La Sapienza", ***110/110 cum laude*** *Rome, Italy*
Thesis: *A quantum approach to the development of force fields for the description of the hydration properties of the Ba^{2+} ion.*
Supervisor: P. D'Angelo

BSc in Chemistry **2013–2016**
Università degli Studi di Roma "La Sapienza", ***110/110 cum laude*** *Rome, Italy*
Thesis: *Structural analysis of metal dihalides with ab initio methods and x-ray absorption spectroscopy.*
Supervisors: P. D'Angelo, G. B. Bachelet

Publications

ORCID: https://orcid.org/0000-0002-0907-0668
Google Scholar: https://scholar.google.com/citations?user=a6-JK2AAAAAJ

- **Caruso**[†] **A.**, Venturin[†] J., Giambagli L., Rolando E., Noé F. & Clementi C. Extending the RANGE of Graph Neural Networks: Relaying Attention Nodes for Global Encoding. *arXiv:2502.13797* (2025).
- Palos E., **Caruso A.** & Paesani F. Consistent density functional theory-based description of ion hydration through density-corrected many-body representations. *J. Chem. Phys.* **159.18**, 181101 (2023).
- Zhai[†] Y., **Caruso**[†] **A.**, Bore[†] S. L. , Luo Z. & Paesani F. A "short blanket" dilemma for a state-of-the-art neural network potential for water: Reproducing experimental properties or the physics of the underlying many-body interactions?. *J. Chem. Phys.* **158.8**, 084111 (2023).
- **Caruso A.**, Zhu X., Fulton J. & Paesani F. Accurate Modeling of Bromide and Iodide Hydration with Data-Driven Many-Body Potentials. *J. Phys. Chem. B* **126.41**, pp. 8266–8278 (2022).
- Gartner III T. E., Hunter K. M., Lambros E., **Caruso A.**, Riera M., Medders G. R., Panagiotopoulos A. Z., Debenedetti P. G. & Paesani F. Anomalies and Local Structure of Liquid Water from Boiling to the Supercooled Regime as Predicted by the Many-Body MB-pol Model. *J. Phys. Chem. Lett.* **13.16**, 3652–3658 (2022).
- **Caruso A.** & Paesani F. Data-driven many-body models enable a quantitative description of chloride hydration from clusters to bulk. *J. Chem. Phys.* **155.6**, 064502 (2021).
- Zhai[†] Y., **Caruso A.**[†], Gao S. & Paesani F. Active learning of many-body configuration space: Application to the Cs^+–water MB-nrg potential energy function as a case study. *J. Chem. Phys.* **152.14**, 144103 (2020).
- Migliorati V., **Caruso A.** & D'Angelo P. Unraveling the hydration properties of the Ba^{2+} aqua ion: the interplay of quantum mechanics, molecular dynamics, and EXAFS spectroscopy. *Inorg. Chem.* **58.21**, 14551–14559 (**2019**).

[†]These authors contributed equally.

Technical Skills

Programming languages: C/C++, Python

Machine learning: PyTorch, JAX, scikit-learn, NetworkX, cuGraph

Molecular dynamics: OpenMM, LAMMPS, Amber, GROMACS, i-Pi, PLUMED

Quantum mechanics: Psi4, MOLPRO, Q-Chem, Gaussian

Data visualization: Blender, Matplotlib, ChimeraX

Other: Bash, LaTeX, HPC interfaces (SLURM, PBS)

Languages: Italian (Native), English (Fluent)

Soft Skills

Creativity, problem solving, and critical thinking: I have written 8 manuscripts (5 first-author) at the forefront of machine learning and computational chemistry.

Teamwork and collaboration: I collaborated with researchers and professors in physics, chemistry, and computer science.

Professionalism and communication: I presented at 5 world-renown seminars and conferences.

Leadership and mentorship: I coordinated multiple projects, mentored graduate and undergraduate students, and assisted in teaching 5 undergraduate and graduate classes.