





# Paolo De Angelis, Ph.D.


PostDoc in Energetics Engineer


 [paolodeangelis.github.io](https://github.com/paolodeangelis)

## Contact

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 [paolo-de-angelis](#)

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## About

 11/11/1993

 Italian


 Male (he/him/his)

## Languages


Italian  *native*

English  *upper intermediate*

## Web presence

 0000-0003-1866-2988

 [jeSYLUUAAAJ](#)

 57212316557

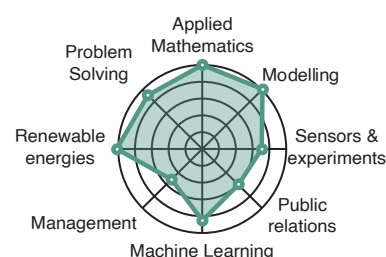
 Paolo-De-Angelis

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 [paolo.de.angelis](#)





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## Professional interests





I am a Postdoctoral Researcher specializing in atomistic modeling for energy storage materials, with expertise spanning thermodynamics, computational chemistry, statistical physics, and machine learning (ML). My research focuses on Li-ion battery (LIB) interface reactions (SEI) using multi-scale approaches. My technical toolkit includes the parametrization of interatomic potentials, from classical to ML-based (MLIP), the use of enhanced sampling methods, and high-throughput DFT and MD simulations on HPC. Beyond technical work, I collaborate with multiple research groups, mentor junior researchers, co-authoring grant proposals, and manage EU project. My short-term goals are to secure a prestigious postdoctoral fellowship to advance my expertise in ML-driven materials study, discovery, and design. In the long term, I aim to establish a robust research profile to apply for funding, such as MSCA, ERC, and Horizon EU, and ultimately securing an academic position.

## Education

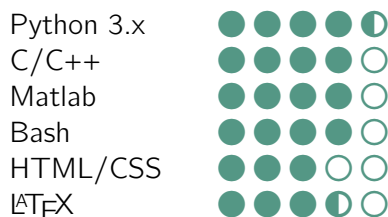
- 2018 - 2022 **PhD in Energetics** [Politecnico di Torino, Italy](#)  
PhD defended on November 2, 2022. Thesis titled "Reactive and Non-Reactive Interface Modelling for Energy Materials".   
Language: *English* Mark: 110L/110
- 2015 - 2017 **MSc in Mechanical Engineering** [Politecnico di Torino, Italy](#)  
University 2nd cycle degree awarded on December 7, 2017. Thesis titled "Simulation of the ensemble and cycle-resolved combustion processes in an NG-H2 engine".   
Language: *English* Mark: 110/110
- 2012 - 2015 **BSc in Mechanical Engineering** [Politecnico di Torino, Italy](#)  
University 1st cycle degree awarded on 9 December 2015. Thesis titled "Quaternion application to 3D roto-translation on simulative environment".   
Language: *Italian* Mark: 107/110
- 2007 - 2012 **Scientific Diploma** [Scientific High School 'B. Rosetti', Italy](#)  
Italian secondary school diploma. (Discussed essay: )  
Language: *Italian* Mark: 84/100

## Experience

- 2023 - now **Affiliated Researcher** [Italian Institute of Technology, Italy](#)  
Close collaboration with Prof. Parrinello's  modeling group  to develop MLIP for investigating lithium-ion mass transport dynamics in LiF inorganic salt incorporating ML tools and enhanced sampling techniques for Free Energy analysis.
- 2022 - now **PostDoc on LIB Modeling** [Politecnico di Torino, Italy](#)  
Postdoctoral researcher in Prof. Chiavazzo's and Prof. Asinari's research group . Developing Reactive FF to investigate the Solid Electrolyte Interface (SEI) in LIB and exploring ML and Graph Neural Networks (GNN) for materials discovery.
- 2020 - 2020 **Visiting at UIC** [University of Illinois at Chicago, USA](#)  
Visiting researcher at the University of Illinois in Chicago (UIC) Mechanical Department, where I developed a multiphysics model of a LIB to train a Deep Neural Network for predicting thermal runaway. (ECS PRiME 2020 Presentation )

## Coding Skills

Proficiency in programming language usage



## Softwares

Short list of know software

### Operating Systems



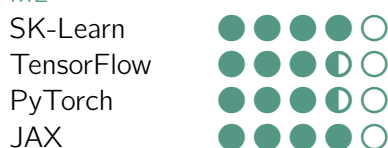
### CFD



### ATOMISTIC



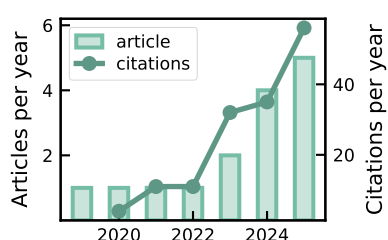
### ML



## Research Output

citations: 151 (Scholar)

h-index: 7 (Scholar)



## Places Lived



## Teaching

- 2024 - now **Machine Learning for energy applications** [01SJFND](#)
- Teaching assistant for 12h lab sessions (in English).
- 2023 - now **Aerosol technology and air quality** [01USDND](#)
- Teaching assistant for 9h lectures (in English).
- 2023 - 2024 **Sistemi a combustione** [06GKYND](#)
- (EN: Combustion systems) Teaching assistant for 24h lab sessions (in Italian).
- 2021 - now **Applicazioni energetiche dei materiali** [02QZSND](#)
- (EN: Advance energy application materials) Teaching assistant for 1.5h lectures and 3h lab sessions (in Italian).
- 2021 - now **Energy storage** [01TVHND](#)
- Teaching assistant for 4.5h lectures (in English).

## Publications

† Equal contribution (co-first) \* Corresponding author

- [1] **P. De Angelis**\* *et al.*, *Exploring Lithium Diffusion in LiF with Machine Learning Potentials: From Point Defects to Collective Ring Diffusion*, (Submitted to "NPJ Comp. Mat."), 2025. DOI: [10.26434/chemrxiv-2025-fv0z1](#).
- [2] **P. De Angelis**, G. Barletta, G. Trezza, P. Asinari, and E. Chiavazzo, "Energy-GNoME: A living database of selected materials for energy applications," *en, Energy and AI*, 2025. DOI: [10.1016/j.egyai.2025.100605](#).
- [3] P. Asinari *et al.*, *Notes on Quantum Computing for Thermal Science*, 2025. DOI: [10.48550/ARXIV.2503.19109](#).
- [4] A. Muhammad†, C. Valero†, **P. De Angelis**†, *et al.*, "From nanoscale to printed products: Multiscale modeling and experimental characterization of graphene-enhanced polylactic acid composites for 3D printing," *en, Composites Part B: Engineering*, 2025. DOI: [10.1016/j.compositesb.2025.112354](#).
- [5] M. Casini, **P. De Angelis**, *et al.*, "Machine Learning and image analysis towards improved energy management in Industry 4.0: A practical case study on quality control," *en, Energy Efficiency*, 2024. DOI: [10.1007/s12053-024-10228-7](#).
- [6] M. Casini†, **P. De Angelis**†, *et al.*, "Current trends on the use of deep learning methods for image analysis in energy applications," *en, Energy and AI*, 2024. DOI: [10.1016/j.egyai.2023.100330](#).
- [7] **P. De Angelis**\*, R. Cappabianca, M. Fasano, P. Asinari, and E. Chiavazzo, "Enhancing ReaxFF for molecular dynamics simulations of lithium-ion batteries: An interactive reparameterization protocol," *en, Scientific Reports*, 2024. DOI: [10.1038/s41598-023-50978-5](#).
- [8] A. Andreozzi *et al.*, "Heat Transfer and Thermal Energy Storage Enhancement by Foams and Nanoparticles," *en, Energies*, 2023. DOI: [10.3390/en16217421](#).
- [9] R. Cappabianca, **P. De Angelis**, M. Fasano, E. Chiavazzo, and P. Asinari, "An Overview on Transport Phenomena within Solid Electrolyte Interphase and Their Impact on the Performance and Durability of Lithium-Ion Batteries," *en, Energies*, 2023. DOI: [10.3390/en16135003](#).
- [10] R. Cappabianca†, **P. De Angelis**†, A. Cardellini, E. Chiavazzo, and P. Asinari, "Assembling Biocompatible Polymers on Gold Nanoparticles: Toward a Rational Design of Particle Shape by Molecular Dynamics," *en, ACS Omega*, 2022. DOI: [10.1021/acsomega.2c05218](#).
- [11] **P. De Angelis** *et al.*, "Data-driven appraisal of renewable energy potentials for sustainable freshwater production in Africa," *en, Renewable and Sustainable Energy Reviews*, 2021. DOI: [10.1016/j.rser.2021.111414](#).

## Hobbies & Interests

Painting & Drawing, Music, Reading, Volunteer Work, Open Source Software, Art Museums, Arduino Projects, Hackathons & Problem Solving, Emerging Technologies, Political Debates, Chess, Cycling, Hiking, Board Games, Cooking, and Traveling.

- [12] **P. De Angelis**, A. Cardellini, and P. Asinari, "Exploring the Free Energy Landscape To Predict the Surfactant Adsorption Isotherm at the Nanoparticle-Water Interface," en, *ACS Central Science*, 2019. DOI: 10.1021/acscentsci.9b00773.

## Conferences & workshops

12/2025	<b>Materials Research Society (MRS)</b> Oral presentation (15') and Poster presentation.	Boston, USA
09/2025	<b>Nanoinnovation</b> Invited presentation (15') and sessions Chairman.	Roma, Italy
09/2025	<b>ICTP - Conference on Frontiers in Atomistic Simulations: from Physics to Chemistry and Biology</b> Invited poster presentation.	Trieste, Italy
10/2024	<b>CECAM - Advances in catalytic reactivity simulations under operando conditions</b> Poster.	Varigotti, Italy
09/2024	<b>European Materials Research Society (E-MRS)</b> Invited presentation (30') and sessions Chairman.	Warsaw, Poland
09/2024	<b>Nanoinnovation</b> Invited presentation (15').	Roma, Italy
09/2024	<b>Symposium on Beyond Li-Ion Batteries - BeLI24</b> Presentation (15').	Padova, Italy
06/2024	<b>23<sup>rd</sup> Symposium on Thermophysical Properties</b> Presentation (15').	Boulder, USA
06/2024	<b>41<sup>st</sup> UIT International Heat Transfer Conference</b> Presentation (15').	Napoli, Italy
05/2022	<b>Materials Research Society (MRS)</b> Presentation (15').	Honolulu, USA
06/2021	<b>15<sup>th</sup> AIGE conference</b> Presentation (15').	Ancona, Italy
10/2020	<b>ECS PRiME</b> Presentation (15').	(Virtual) Honolulu, USA
03/2020	<b>American Physical Society (APS)</b> Presentation (15').	(Virtual) Denver, USA
06/2019	<b>CECAM - Materials Simulation Days</b> Poster.	Mainz, Germany

## References

### Professor **Pietro Asinari**

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📍 *Politecnico di Torino, 10129, Torino TO, Italy*

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