Antonios P. Sarikas

Computational Chemist

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https://adosar.github.io/
adosar
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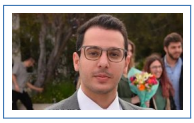
3 January 2000



If the implementation is easy to explain, it may be a good idea.

Education

2024–TBA	PhD, Physical & Computational Chemistry, Department of Chemistry, University of Crete
2022–2024	MSc, Physical & Computational Chemistry, Department of Chemistry, University of Crete *9.86* (Excellent)
2018–2022	BSc, Chemistry, Department of Chemistry, University of Crete *8.64* (Excellent) **First of the class — obtained in 3.5/4.0 years**

Master thesis

Title	From Potential Energy Surface to Gas Adsorption via Deep Learning
Supervisor	George E. Froudakis
Description	Developing a deep learning based method for predicting gas adsorption in porous materials using 3D energy images.
Repository	`https://github.com/adosar/master_thesis`

Bachelor thesis

Title	Screening of MOFs for H_2 Storage via Machine Learning
Supervisor	George E. Froudakis
Description	Developing a machine learning based method for fast screening of large databases, in order to identify top performing MOFs for hydrogen storage.

Scholarships – Awards – Highlights

2025	Best MSc Thesis Award, Hellenic Society for the Science and Technology of Condensed Matter
2025	Ranked 9th in Scientific Reports' 2024 Materials Science Top 100. "Gas adsorption meets deep learning: voxelizing the potential energy surface of metal-organic frameworks".
2024	Postgraduate Fellowship, Independent Power Transmission Operator S.A. Fellowship
2024	Postgraduate Fellowship, Maria Michail Manasaki Bequest Fellowship
2023	Chatzimarinaki Award, Department of Chemistry, University of Crete
2022	Undergraduate Scholarship, Stamatiou Foundation
2021	Undergraduate Scholarship, Stamatiou Foundation
2020	Undergraduate Scholarship, Stamatiou Foundation

¶ Publications

[1] Aydin Ozcan, François-Xavier Coudert, Sven M. J. Rogge, Greta Heydenrych, Dong Fan, Antonios P. Sarikas, Seda Keskin, Guillaume Maurin, George E. Froudakis, Stefan Wuttke, and Ilknur Erucar. "Artificial Intelligence Paradigms for Next-Generation Metal–Organic Framework Research". In: *Journal of the American Chemical Society* (June 2025). DOI: 10.1021/jacs.5c08214.

[2] Antonios P. Sarikas, Konstantinos Gkagkas, and George E. Froudakis. "Gas adsorption meets deep learning: voxelizing the potential energy surface of metal-organic frameworks". In: *Scientific Reports* 14.1 (Jan. 2024). DOI: 10.1038/s41598-023-50309-8.

[3] Antonios P. Sarikas, Konstantinos Gkagkas, and George E. Froudakis. "Gas adsorption meets geometric deep learning: points, set and match". In: *Scientific Reports* 14.1 (Nov. 2024), p. 27360. DOI: 10.1038/s41598-024-76319-8.

[4] Antonios P. Sarikas, George S. Fanourgakis, and George E. Froudakis. "Metal-organic frameworks in the age of machine learning". In: *Reticular Chemistry and Applications*. De Gruyter, Jan. 2023. DOI: 10.1515/9781501524721.

[5] Antonios P. Sarikas, George S. Fanourgakis, Konstantinos Gkagkas, and George E. Froudakis. "Comparison of machine learning approaches for the identification of top-performing materials for hydrogen storage". In: *Sustainable Chemistry for the Environment* 5 (Mar. 2023), p. 100056. DOI: 10.1016/j.scenv.2023.100056.

[6] Antonios P. Sarikas, George S. Fanourgakis, Emmanuel Tylianakis, Konstantinos Gkagkas, and George E. Froudakis. "Comparison of Energy-Based Machine Learning Descriptors for Gas Adsorption". In: *The Journal of Physical Chemistry C* (Oct. 2023). DOI: 10.1021/acs.jpcc.3c04223.

Peer-review activities

2025 Reviewer for *Scientific Reports*

2025 Reviewer for *Communications Chemistry*

2024 Reviewer for *Journal of Cheminformatics*

</> Software

AIdsorb — python package for deep learning on molecular point clouds

- Homepage
- Documentation

AIdsorb-online — A web app for predicting properties of porous materials via deep learning

- Click to open the app

moXελ — python package for parallel calculation of energy voxels

- Homepage
- Documentation

RetNet — A 3D ConvNet for Reticular Chemistry

- Homepage

Presentations

2024 COST Action EU4MOFs, Istanbul
2023 Chatzimarinaki Seminar, Heraklion
2023 1st Mediterranean Conference on Porous Materials, Rethymnon
2022 Chatzimarinaki Seminar, Heraklion
2022 XXXVI Pan-Hellenic conference on Solid-State Physics and Materials Science, Heraklion

Workshops

2024 Computational Materials Science, University of Thessaly, Online
2023 Computational Materials Science, National Kapodistrinan University of Athens, Online
2022 Computational Materials Science, University of Ioannina, Online
2021 Computational Materials Science, University of Patras, Online
2021 DCMS Materials 4.0 Summer School, TU Dresden, Online

Computer skills

Operating Systems: Fedora Linux, Ubuntu, Windows
Programming Languages: Python, Fortran
Markup Languages: LaTeX, Markdown
Other Tools: Git, Github, Sphinx, Vim, MSOffice

Working experience

2025 Coordinator for 3C Summer School V2, Department of Chemistry, University of Crete
2023, 2025 Teaching assistant on the Laboratory of Physical-Chemistry II, Department of Chemistry, University of Crete
2023, 2024 Teaching assistant on the Laboratory of Physical-Chemistry I, Department of Chemistry, University of Crete

Languages

English: Proficiency, University of Michigan
Greek: Native language