

# Antonios P. Sarikas

Computational Chemist

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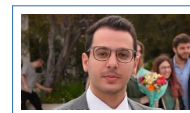
🌐 [adosar.github.io/](https://adosar.github.io/)

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3 January 2000



*Βελτίων ἢ ἐξ ἐλαττόνων.*

## 🎓 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.
- Document [Click here to access it](#)

## 📄 Bachelor thesis

- Title Screening of MOFs for H<sub>2</sub> 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 **Excellence Award**, "Professor Zoe Dimitriadis Prize", University of Crete
- 2025 **Best MSc Thesis Award** (3rd place), Federation of European Materials Societies
- 2025 **Postgraduate Fellowship**, Vasileios Apollon Anagnostakis Bequest Fellowship
- 2025 **Best MSc Thesis Award** (1st place), Hellenic Society for the Science and Technology of Condensed Matter
- 2025 **Paper featured in *Nature Portfolio Nobel Prize in Chemistry 2025***. "Gas adsorption meets deep learning: voxelizing the potential energy surface of metal-organic frameworks"
- 2025 **Paper 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 Manassaki Bequest Fellowship

- 2023 **Chatzimarini Award**, Department of Chemistry, University of Crete  
2022 **Undergraduate Scholarship**, Stamatiou Foundation  
2021 **Undergraduate Scholarship**, Stamatiou Foundation  
2020 **Undergraduate Scholarship**, Stamatiou Foundation

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## Publications

- [1] Alexios P. Drosos, Antonios P. Sarikas, and George E. Froudakis. "Predicting Hydrogen Storage in MOFs: Representation Matters". In: *International Journal of Hydrogen Energy* (May 2026). Under revision.
- [2] Antonios P. Sarikas, Konstantinos Gkagkas, and George E. Froudakis. "RetNeXt: A Pretrained Model for Transfer Learning Across the MOF Adsorption Space". In: *Journal of Chemical Information and Modeling* (Feb. 2026). doi: 10.1021/acs.jcim.5c02698.
- [3] 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.
- [4] 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.
- [5] 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.
- [6] 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. 2024), p. 100056. doi: 10.1016/j.scenv.2023.100056.
- [7] 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.
- [8] 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.



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## Peer-review activities

- 2026 Reviewer for *npj Artificial Intelligence*  
2026 Reviewer for *npj Computational Materials*  
2025 Reviewer for *Scientific Reports*  
2025 Reviewer for *Communications Chemistry*  
2024 Reviewer for *Journal of Cheminformatics*

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## Software

  package for deep learning on molecular point clouds

-  Homepage
-  Documentation



A web app for evaluating pocket-ligand fitness via machine learning

- Click to open the app

**Aldorb-online**

A web app for predicting properties of porous materials via deep learning

- Click to open the app



python™ package for parallel calculation of energy voxels

- Homepage
- Documentation

**RetNeXt**

Deep learning on 3D energy images of porous materials

- Homepage

**RetNet**

A 3D ConvNet for Reticular Chemistry

- Homepage

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## Presentations

- 2025 Memorial seminar in honor of Dr. Chatzimarini, Heraklion
- 2025 Young Scientist Symposium (EuroMOF2025), Heraklion
- 2025 EuroMOF2025, Heraklion
- 2025 FEMS Masters Thesis Award, Granada
- 2025 FEMS EUROMAT 2025, Granada
- 2025 3C Summer School V2, Heraklion
- 2025 HSSTCM Masters Thesis Award, Online
- 2024 COST Action EU4MOFs, Istanbul
- 2023 Memorial seminar in honor of Dr. Chatzimarini, Heraklion
- 2023 1st Mediterranean Conference on Porous Materials, Rethymnon
- 2022 Memorial seminar in honor of Dr. Chatzimarini, Heraklion
- 2022 XXXVI Pan-Hellenic conference on Solid-State Physics and Materials Science, Heraklion

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## Workshops

- 2024 Computational Materials Science, University of Thessaly, Online
- 2023 Computational Materials Science, National Kapodistrian 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

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## Computer skills

- Operating Systems  
Fedora Linux, Ubuntu, Windows

Programming Languages Python, Fortran  
Markup Languages  $\LaTeX$ , Markdown  
Other Tools Git, Github, Sphinx, Vim, MSOffice

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## 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

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## Languages

English Proficiency, University of Michigan  
Greek Native language