

# Antonios P. Sarikas

Computational Chemist

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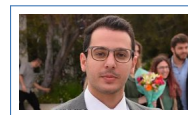
🌐 <https://adosar.github.io/>

🐙 adosar

🔑 Zv2UkOAAAAAJ

🆔 0009-0008-8420-927X

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](https://github.com/adosar/master_thesis)

## 🎓 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 Chemistry 2025 Collection*. "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 Manasaki 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

## 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



 python™ package for deep learning on molecular point clouds


- [!\[\]\(97faa0168e491544be255cfcab218e9b\_img.jpg\) Homepage](#)
- [!\[\]\(b2166b76608b8499cffc130bf1b1fe60\_img.jpg\) Documentation](#)

### **Aldorb-online**

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

- [!\[\]\(c50c8b7b2cc2cf9ff925edec0ee94c0d\_img.jpg\) Click to open the app](#)



 python™ package for parallel calculation of energy voxels












- [!\[\]\(adb0331d22f78481623cc605df40612a\_img.jpg\) Homepage](#)
- [!\[\]\(7e3a264c08e10137510d1aa76522412b\_img.jpg\) Documentation](#)

**RetNet** A 3D ConvNet for Reticular Chemistry

[🔗](#) [🏠 Homepage](#)

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## Presentations

-  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 Chatzimarinkaki Seminar, Heraklion
-  2023 1st Mediterranean Conference on Porous Materials, Rethymnon
-  2022 Chatzimarinkaki Seminar, 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