

# Antonios P. Sarikas

Computational Chemist

✉ [antonios.sarikas@gmail.com](mailto:antonios.sarikas@gmail.com)

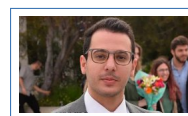
🌐 <https://adosar.github.io/>

🐙 adosar

🔑 Zv2Uk0AAAAAJ

🆔 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 Ranked 9th in Scientific Reports' 2024 Materials Science Top 100. "Gas adsorption meets deep learning: voxelizing the potential energy surface of metal-organic frameworks".
- 2025 Best MSc Thesis Award, Hellenic Society for the Science and Technology of Condensed Matter
- 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

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## Publications

- [1] 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.
- [2] 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.
- [3] 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.
- [4] 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.
- [5] Antonios P. Sarikas, George S. Fanourgakis, Emmanuel Tylanakis, 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.

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## Peer-review activities

- 2025 Reviewer for *Scientific Reports*
- 2025 Reviewer for *Communications Chemistry*
- 2024 Reviewer for *Journal of Cheminformatics*

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## Software



 python™ package for deep learning on molecular point clouds

- [!\[\]\(c6a8736a601a632e2c96605cf66055ed\_img.jpg\) Homepage](#)
- [!\[\]\(64ef2b19d70b31fbbfce0e0e2aa3d7b4\_img.jpg\) Documentation](#)

**Aldorb-online** A web app for predicting properties of porous materials via deep learning

- [!\[\]\(3211b5d1d968fc1665909b34f9f16010\_img.jpg\) Click to open the app](#)



 python™ package for parallel calculation of energy voxels



- [!\[\]\(b6d55d0b173caf9b2505126db01e6158\_img.jpg\) Homepage](#)
- [!\[\]\(12811766810e4126d2bed4d8c0808e60\_img.jpg\) Documentation](#)




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

- [!\[\]\(9c2e8d1b5bd77cb5c9f83b7a9cff79fd\_img.jpg\) Homepage](#)

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## Presentations

-  2024 COST Action EU4MOFs, Istanbul
-  2023 Chatzimariniaki Seminar, Heraklion

-  2023 1st Mediterranean Conference on Porous Materials, Rethymnon
-  2022 Chatzimarinki 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 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

## 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