

Antonios P. Sarikas

Computational Chemist

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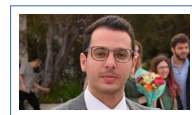
🌐 <https://adosar.github.io/>

🐙 [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

🎓 Bachelor thesis

- Title Screening of MOFs for H₂ 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 Postgraduate Fellowship, Vasileios Apollon Anagnostakis Bequest Fellowship
- 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 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.sceenv.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

- [!\[\]\(4e333a6106fc298d0ae6dff272a736ef_img.jpg\) Homepage](#)
- [!\[\]\(97089f8e07e24e31baa67366e358a709_img.jpg\) Documentation](#)

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

- [!\[\]\(97faa0168e491544be255cfcab218e9b_img.jpg\) 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

- [!\[\]\(adb0331d22f78481623cc605df40612a_img.jpg\) Homepage](#)

Presentations

-  2024 COST Action EU4MOFs, Istanbul
-  2023 Chatzimariniaki Seminar, Heraklion
-  2023 1st Mediterranean Conference on Porous Materials, Rethymnon
-  2022 Chatzimariniaki 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