# Antonios P. Sarikas

# Computational Chemist





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 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 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

- Antonios P. Sarikas, Konstantinos Gkagkas, and George E. Froudakis. "RetNeXt: A pretrained model for [1] transfer learning across the MOF adsorption space". In: Journal of Chemical Information and Modeling (Submitted) (Oct. 2025).
- [2] 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.
- 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, 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.
- [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. 2024), p. 100056. poi: 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.
- 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. poi: 10.1515/ 9781501524721.

#### Peer-review activities

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





dsorb python package for deep learning on molecular point clouds

O Homepage

Documentation

A web app for predicting properties of porous materials via deep learning Aldsorb-online O Click to open the app



 $\bigcap$   $\epsilon\lambda$  python package for parallel calculation of energy voxels

O Homepage

Documentation

RetNet A 3D ConvNet for Reticular Chemistry

O 🞧 Homepage

#### 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 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
- Computational Materials Science, University of Patras, Online 2021
- DCMS Materials 4.0 Summer School, TU Dresden, Online 2021

#### Computer skills

Fedora Linux, Ubuntu, Windows Operating

Systems

Programming Python, Fortran

Languages

Markup LTEX, Markdown

Languages

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

# ■ A Languages

English Proficiency, University of Michigan

Greek Native language