# Antonios P. Sarikas

Chemist



If the implementation is easy to explain, it may be a good idea.

#### Education

2022–2024 Master of Science, Physical Chemistry, Department of Chemistry, University of Crete 9.86 (Excellent)

2018–2022 Bachelor of Science, 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 the 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.

Repository 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

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

- [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.
- 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.





dsorb 🍦 python package for deep learning on molecular point clouds

- Homepage
- ■ Documentation
- Online app for predicing properties of porous materials



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

- Homepage
- E Documentation

RetNet A 3D ConvNet for Reticular Chemistry

Homepage

## Presentations – Posters

- 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

- 2023 Computational Materials Science, National Kapodistrinan 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

Systems

Operating Fedora Linux, Ubuntu, Windows

Programming Python, Fortran

Languages

Markup LATEX, Markdown

Languages

Other Tools Git, Github, Sphinx, Vim, MSOffice

## **Working** experience

2023, 2024 Teaching assistant on the Laboratory of Physical-Chemistry I, Department of Chemistry, University of Crete

2023 Teaching assistant on the Laboratory of Physical-Chemistry II, Department of Chemistry, University of Crete

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English Proficiency, University of Michigan

Greek Native language