

Antonios P. Sarikas

Chemist

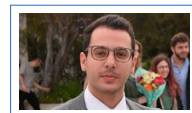
✉ antonios.sarikas@gmail.com

🌐 <https://adosar.github.io/>

👤 adosar

🔗 Zv2Uk0AAAAAJ

3 January 2000



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.

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

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
2021–2022 Undergraduate scholarship, Stamatiou Foundation
2020–2021 Undergraduate scholarship, Stamatiou Foundation
2019–2020 Undergraduate scholarship, Stamatiou Foundation


Publications

Published

- [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). ISSN: 2045-2322. 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. ISSN: 2045-2322. 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. ISSN: 2949-8392. DOI: 10.1016/j.scenv.2023.100056.
- [5] 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.

Software development



 python package for deep learning on molecular point clouds

- [Source code](#)
- [Documentation](#)
- [Online app](#)



 python package for parallel calculation of energy voxels

- [Source code](#)
- [Documentation](#)

Presentations – Posters

- [Chatzimarini Seminar 2023, Heraklion, November 2023](#)
- [1st Mediterranean Conference on Porous Materials, Rethymnon, May 2023](#)
- [Chatzimarini Seminar 2022, Heraklion, November 2022](#)
- [XXXVI Pan-Hellenic conference on Solid-State Physics and Materials Science, Heraklion, September 2022](#)

Workshops

- [Computational Materials Science, National Kapodistrian University of Athens, Online, December 2023](#)

- Computational Materials Science, University of Ioannina, Online, December 2022
- Computational Materials Science, University of Patras, Online, December 2021
- DCMS Materials 4.0 Summer School, TU Dresden, Online, August 2021

Working experience

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

Languages

- English Proficiency, University of Michigan
- Greek Native language

Computer skills

- Operating Systems Linux, Windows
- Programming Languages Python, Fortran
- Other \LaTeX , MSOffice