Antonios P. Sarikas

Chemist

+30 694 641 7140
antonios.sarikas@gmail.com
https://adosar.github.io/
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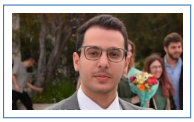
3 January 2000



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

Education

2022–2024 Master of Science, Computational 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 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

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

2021–2022 Undergraduate scholarship, Stamatiou Foundation

2020–2021 Undergraduate scholarship, Stamatiou Foundation

2019–2020 Undergraduate scholarship, Stamatiou Foundation

Publications

Published

[1] 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. ISSN: 2949-8392. DOI: 10.1016/j.scenv.2023.100056.

[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). ISSN: 2045-2322. DOI: 10.1038/s41598-023-50309-8.

[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, 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

AIdsorb — python package for deep learning on molecular point clouds

- Source code
- Documentation

moXελ — python package for parallel calculation of energy voxels

- Source code
- Documentation

Presentations – Posters

- Chatzimarinaki Seminar 2023, Heraklion, November 2023
- 1st Mediterranean Conference on Porous Materials , Rethymnon, May 2023
- Chatzimarinaki Seminar 2022, Heraklion, November 2022
- XXXVI Pan-Hellenic conference on Solid-State Physics and Materials Science, Heraklion, September 2022

Workshops

- Computational Materials Science, National Kapodistrinan 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