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.
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

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.

[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

AIdsorb python package for deep learning on molecular point clouds

- Homepage
- Documentation

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

- Click to open the app

moXελ python package for parallel calculation of energy voxels

- Homepage
- 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

Operating Systems	Fedora Linux, Ubuntu, Windows
Programming Languages	Python, Fortran
Markup Languages	LaTeX, Markdown
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

Languages

English	Proficiency, University of Michigan
Greek	Native language