

# Antonios P. Sarikas

Chemist

+30 694 641 7140

✉ antonios.sarikas@gmail.com

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3 January 2000



## 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<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

- 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, 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.sceenv.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.

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## Presentations – Posters

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

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## Software development



 package for parallel calculation of energy voxels

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## 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

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## Working experience

- 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

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## Languages

English Proficiency, University of Michigan

Greek Native language

 Computer skills

Operating Systems Linux, Windows

Programming Languages Python, Fortran

Other  $\LaTeX$ , MSOffice