

Panagiotis Krokidas, PhD

IF Marie Skłodowska-Curie postdoc fellow (as of May 1st, 2020)
Membranes and Materials for Environmental Separations
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I am a physicist whose main scientific interests lie in the field of novel **nanoporous and microporous materials** design for highly challenging and environmentally urgent separations. My research approaches are computational and lie mainly on the molecular level: **molecular dynamics, transition state theory, Monte Carlo, Widom test particle insertion** and **force field development**. I am also a skilled programmer with experience in **FORTRAN** and **Python** programming, and **bash scripting** languages, among others. Moreover, I am highly interested in big data analysis and **Machine Learning** methods. This interest shaped a project in my mind which was **awarded** in 2020 with the prestigious **Marie Skłodowska-Curie grant** (2019 cycle, MSCA-IF-EF-RI panel, with no 894585 and project acronym SmartDeZign). The project's theme is the development of a design tool of highly selective metal-organic frameworks (MOFs) membranes with **Machine Learning methods**.

Machine Learning and Big Data analysis morphed from an interesting and a necessary tool for my project's needs into a big love of mine. Dr. Giannakopoulos, who is an expert in ML, is one of the supervisors of my IF-MSCA funded project, and he is mentoring me in ML matters through weekly meetings. Moreover, I have finished a wide series of relevant courses, and recently I received the **Data Science Professional** Certificate from IBM, in Coursera (see section *Further Education: Courses, Workshops, Tutorials*, at the end of the document).

PROFFESIONAL EXPERIENCE

01/05/2020 - present	Postdoctoral research and Marie Curie fellow – Membranes and Materials for Environmental Separations, Institute of Nanoscience and Nanotechnology, NCSR "Demokritos"
01/10/2019-31/04/2020	Postdoctoral researcher - Molecular Thermodynamics and Modelling of Materials Laboratory, Institute of Nanoscience and Nanotechnology, NCSR "Demokritos"
01/09/2014 - 01/07/2019	Postdoctoral research associate – Chemical Engineering, Texas A&M University at Qatar
15/10/2012 - 30/03/2014	Postdoctoral scientist - Department of Materials and Environmental Chemistry, Stockholm University

RESEARCH CAREER GAP

(10/2011 - 7/2012)

Obligatory military service

EDUCATION

8/2008 - 10/2011	PhD - Department of Materials Science, University of Patras, University of Patras & FORTH-ICEHT, Patras, Greece.
03/11/2005 - 17/8/2008	MS - Department of Materials Science, University of Patras & Foundation for Research & Technology Hellas, Institute of Chemical Engineering & High Temperature Chemical Processes (FORTH-ICEHT), Patras, Greece.
15/09/1999 - 25/10/2005	BS - Department of Physics, University of Patras, Patras, Greece

BOOK CHAPTERS

1. I.G Economou, P. Krokidas, V.K. Michalis, O.A. Moulτος, I.N. Tsimpanogiannis and N. Vergadou, "The Role of Molecular Thermodynamics in Developing Industrial Processes and Novel Products that Meet the Needs for a Sustainable Future", In *The Water-Food-Energy Nexus: Processes, Technologies, and Challenges*, I.M. Mujtaba, R. Srinivasan, N.O. Elbashir, Eds., CRC Press, US (2017).

PEER-REVIEWED PUBLICATIONS

1. **P.G. Krokidas**, E.D. Skouras, B. Nikolakis and V.N. Burganos, Simulated annealing effects on Na-FAU crystal reconstruction and sorption efficiency, *Mol. Simulat.*, **2008**, 34, 10-15, 1299-1309.
2. **P.G. Krokidas**, E.D. Skouras, B. Nikolakis and V.N. Burganos, Lattice dynamics simulation of thermal contraction of faujasites, *J. Phys. Chem. C*, **2010**, 114 (51), 22441–22448.
3. **P.G. Krokidas**, B. Nikolakis and V.N. Burganos, Heating and sorption effects on silicalite-1 unit cell size and geometry, *Micropor. Mesopor. Mat.*, **2012**, 155, 1, 65–70.
4. O. Cheung, Z. Bacsik, **P. Krokidas**, A. Mace, A. Laaksonen, N. Hedin, K⁺ exchanged zeolite ZK-4 as a highly selective sorbent for CO₂, *Langmuir*, **2014**, 30(32). 9682-9690
5. **P. Krokidas**, M. Castier, S. Moncho, E. Brothers, I.G. Economou, Molecular simulation studies of the diffusion of methane, ethane, propane and propylene in ZIF-8, *J. Phys. Chem. C*, **2015**, 119 (48), 27028-27037
6. **P. Krokidas**, M. Castier, S. Moncho, D. Sredojevic, E. Brothers, H.T. Kwon, H-K, Jeong, H-K, J.S. Lee and I.G. Economou, ZIF-67 Framework: A Promising New Candidate for Propylene/Propane Separation. Experimental Data and Molecular Simulations, *J. Phys. Chem. C* **2016**, 120, 8116-8124
7. **P. Krokidas**, M. Castier, I.G. Economou, A Computational Study of ZIF-8 and ZIF-67 Performance for Separation of Gas Mixtures, *J. Phys. Chem. C* **2017**, 121, 17999-18011

8. **P. Krokidas**, S. Moncho, E. Brothers, M. Castier, and I.G. Economou, Tailoring the gas separation efficiency of metal organic framework ZIF-8 through metal substitution: a computational study, *Phys. Chem. Chem. Phys.* **2018**, 20, 4879-4892
9. A. Mamoon, **P. Krokidas** and I.G. Economou, CO₂ selective metal organic framework ZIF-8 modified through ionic liquid encapsulation: a computational study, *J. Comput. Sci.* **2018**, 27, 183-191
10. **P. Krokidas**, S. Moncho, E. Brothers, M. Castier, H-K, Jeong and I.G. Economou, On the efficient separation of gas mixtures with the mixed-linker zeolitic-imidazolate framework-7-8, *ACS Appl. Mater. Interfaces*, **2018**, 10, 39631-39644
11. A. Mamoon, **P. Krokidas**, S. Moncho, K. Kakosimos, E. Brothers, and I.G. Economou, Computational investigation of the performance of ZIF-8 with encapsulated ionic liquids towards CO₂ capture, *Mol. Phys.* **2019**, 1-15
12. **P. Krokidas**, S. Moncho, E. Brothers and I.G. Economou, Defining New Limits in Gas Separations Using Modified ZIF Systems, *ACS Appl. Mater. Interfaces*, **2020**, 12, 20536-20547
13. A. Mamoon, **P. Krokidas** and I.G. Economou, Encapsulation of [bmim+][Tf₂N-] in different ZIF-8 metal analogues and evaluation of their CO₂ selectivity over CH₄ and N₂ using molecular simulation, *Mol. Syst. Des. Eng.*, **2020**, 5, 1230-1238
14. O. Cheung, B. Zoltan, N. Fil, **P. Krokidas**, D. Wardecki and N. Hedin, Selective adsorption of CO₂ on zeolites NaK-ZK-4 with Si:Al of 1.8 – 2.8, *ACS Omega* **2020**, 5, 25371-25380
15. F. Hillman, M. R. A. Hamid, **P. Krokidas**, S. Moncho, E. Brothers, I.G. Economou, H.-K. Jeong, Delayed Linker Addition (DLA) Synthesis for Hybrid SOD ZIFs with Unsubstituted Imidazolate Linkers for Propylene/Propane and n-Butane/i-Butane Separations, *Angew. Chem.*, **2021**, 133, 10191-10199

PUBLICATIONS UNDER PROGRESS

1. **P. Krokidas**, S. Karozis, S. Moncho, E. Brothers, G. Giannakopoulos, M. Kainourgiakis, I.G. Economou, T. Steriotis, *under preparation*

PARTICIPATION IN CONFERENCES

1. May 2007 6thInternational Scientific Conference of Chemical Engineering, 2007 (Oral presentation: Investigation of gas sorption and separation in zeolites using molecular simulation techniques)
2. November 2007 3rdInternational Conference of Porous Materials (oral presentation: Molecular simulation of sorption and separation in hydrated and nonhydrated zeolites)
3. July 2007 4th International Zeolite Membrane Meeting (poster: Investigation of Gas Sorption and Separation in Zeolites Using Molecular Simulation Techniques)
4. May 2008 4th Conference on Engineering with Membranes, EWM 2008 (poster: Simulation of Sorption and Transport in Faujasites for Gas Separation Tailoring)
5. June 2009 6thInternational Scientific Conference of Chemical Engineering (oral presentation: Reconstruction of zeolitic structures with the use of energy and entropy minimization techniques)
6. October 2009 4th International Conference of Porous Materials (oral presentation: Reconstruction of nanoporous faujasite structures with the use of energetic and entropic criteria of lattice optimization)
7. May 2010 5thInternational Zeolite Membrane Meeting (oral presentation: Temperature and adsorption effects on zeolite structure and elastic properties using molecular simulations)
8. July 2011 International Congress on Membranes and Membrane Processes (presenting oral: Conduction in fuel cell membranes impregnated with ionic liquids and zeolite crystals)
9. November 2013 2013 AIChE Annual Meeting (participation in oral presentation: Carbon Dioxide Separation Using Highly Selective Narrow Pore Zeolite ZK-4)
10. November 2015 X IberoAmerican Conference on Phase Equilibria and Fluid Properties for Process Design, Alicante (oral presentation: Modification of ZIF-8 structures: the effect of metal atom exchange on structural and separation properties,)
11. June 2015 15th AIChE Annual Meeting (participation in oral presentation: Heteroepitaxially-Grown Zeolitic Imidazolate Framework Membranes with Unprecedented Propylene/Propane Separation Performance)

12. June 2016 14th International Conference on Inorganic Membranes (2016), Atlanta (oral presentation: Modification and tailoring of the ZIF-8 framework for various separations: force-field development and molecular simulations)
13. September 2017 Thermodynamics 2017, Edinburgh, (poster: Modifying ZIF-8 framework through metal substitution towards separation improvement of gas mixtures)
14. October 2017 The Second International Computational Science and Engineering Conference (oral presentation: CO₂ selective ZIF frameworks modified through ionic liquid encapsulation)
15. February 2018 The Eleventh International Conference on Thermal Engineering Theory and Applications (oral presentation: Modification and tailoring of the ZIF-8 framework for various separations: force-field development and molecular simulations)
16. June 2018 15th International Conference on Inorganic Membranes (oral presentation: Structural modification techniques for tailoring ZIFs for gas separation: a computational study)
17. September 2018 8th International Symposium on Molecular Thermodynamics and Molecular Simulation (oral presentation: Molecular design and prediction of structure and physical properties of complex systems of importance to the oil and gas industry)
18. October 2018 2018 AIChE Annual Meeting (oral presentation: Control over the Gas Separation Range of Zeolitic Imidazolate Framework-8 Based Membranes: Metal Replacement and Linkage Exchange)
19. December 2020 12th International Congress on Membranes and Membrane Processes (oral presentation: Molecular level design of zeolitic-imidazolate framework membranes for the separation of light gases)
20. July 2021 31st European Symposium on Applied Thermodynamics (oral presentation: Physics Driven Machine Learning Model for the Design of Highly Selective Zeolitic-imidazolate Framework)
21. September 2021 4th European Conference on Metal Organic Frameworks and Porous Polymers (oral presentation: Molecular Level Design of Zeolitic-imidazolate Framework Membranes for the Separation of Light Gases)
22. November 2021 AIChE Annual Meeting (co-author of oral presentation: A Novel Machine Learning Model for the Accurate Design of Highly Selective Zeolitic-Imidazolate Frameworks)

EDITORIAL DUTIES

Reviewer for Chemistry of Materials, Journal of Physical Chemistry, Fluid Phase Equilibria, ACS Applied Materials & Interfaces, Brazilian Journal of Chemical Engineering

TEACHING EXPERIENCE

Instructor of Molecular Simulations Techniques and Scientific Computing, in Molecular Thermodynamics and Simulation Laboratory, Texas A&M University at Qatar:

- Instructing graduate students on simulation techniques (molecular dynamics and Monte Carlo), molecular visualization approaches.
- Instructing graduate students on scientific computing, programming, bash scripting and Linux usage
- Mentoring undergraduate students on introductory research projects

Mentoring of Master Students in Molecular Thermodynamics and Simulation Laboratory, Texas A&M University at Qatar:

- Amro Mohamed Mamoon (2018-2020) a project around sorption, storage and separation of CO₂ related mixtures in prototype Zeolitic-Imidazolate Frameworks. Master Thesis Title: CO₂ Selective Zeolitic Imidazolate Frameworks (ZIFs) Modified Through Ionic Liquid Encapsulation: A Computational Study.
- Laya Roustazadeh (2021-) a project around dehumidification membranes for air-cooling process

FUNDED PROJECTS I WORKED IN

10.2005-10.2011 – as a Master and PhD student, under the supervision of Dr. Vasilis Burganos (Institute of Chemical Engineering Sciences - ICE-HT of Foundation for Research and Technology - FORTH)

- Expanding membrane macroscale applications by exploring nanoscale material properties, NanoMemPro, Network of Excellence, FP6 European Project (Project ID: 500623)
- ZEOCELL, FP7 European collaborative projects (Grant Agreement no: 209481)

10.2012-04.2014 – as a postdoctoral researcher, under the supervision of assoc. Professor Niklas Hedin (Department of Materials and Environmental Chemistry, Stockholm University)

- Process simulation of biogas upgrading with swing adsorption technologies (Richert Foundation – R&D Grant)

09.2014-07.2019 – as a postdoctoral researcher, under the supervision of Professor Ioannis G. Economou (Chemical Engineering, Texas A&M University at Qatar)

- 2014-2017 Design and Optimization of Highly Productive Zeolitic Imidazolate, ZIF-8, Membranes for Industrial Propylene/Propane Separations (NPRP No.: NPRP 7 - 042 - 2 - 021)
- 2017-2019 Advance Design Methods for Gas Separation Membranes (Responsive Research Grant)

09.2019-05.2020 – as a postdoctoral researcher, under the supervision of Dr. Ioannis G. Economou (Institute of Nanoscience and Nanotechnology, National Center for Scientific Research “Demokritos”)

05.2020-present – as a postdoctoral researcher and Marie Curie fellow, under the supervision of Dr. Theodore Steriotis

(Institute of Nanoscience and Nanotechnology, National Center for Scientific Research “Demokritos”)

- Smart Design Tool of High Performing ZIF Membranes for Important CO₂-related Separations (SmartDeZIgn)

WRITING OF PROPOSALS

Title	Year	Funding Scheme
Adsorbents for the separation of carbon dioxide from flue gas mixtures	2013	Carl Trygger foundation (Sweden), Not Approved
Advance Methods for Gas Separation Membranes	2016	Responsive Research Grant (Texas A&M), Approved
Tunable Molecular Sieve Hybrid Zeolitic-Imidazolate Framework Hollow Fiber Membranes for Custom Separations of Challenging Gas Mixtures	2018	Qatar Foundation (NPRP no: NPRP 11S-0109-180240), Approved
Innovative Asymmetric Mixed Matrix Hollow Fiber Membranes for Gas Mixture Separation	2019	Qatar Foundation (NPRP no: NPRP 12S-0209-190064), Approved
Design of novel metal-organic frameworks for membrane-based gas separations	2019	2 nd call Hellenic Foundation for research & Innovation (H.F.R.I.) research projects for the support of postdoctoral researchers, not Approved
Smart Design Tool of High Performing ZIF Membranes for Important CO ₂ -related Separations (SmartDeZIgn)	2020	H2020, Marie Skłodowska-Curie Actions Individual Fellowships (IF), Approved (no 894585 and project acronym <i>SmartDeZIgn</i>)

Low-carbon pathways for industrial CO ₂ utilisation, transport, and storage (LowCarbonPath)	2020	H2020, Innovation Actions (IA), not Approved
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RESEARCH SKILLS AND INTERESTS

- Process modeling:
 - simulation of flow through porous media, modeling of units for separation processes and capture of gases. Simulation and optimization of PSA/rPSA, vacuum PSA units for gas separation
- Atomistic scale simulations:
 - Sorption, storage and diffusion of gases in ionic liquids and nanoporous solids (zeolites, MOFs, ZIFs). Calculation of sorption properties (adsorption isotherms, isosteric heats of adsorption) with Monte Carlo and Widom test particle theory. Gas diffusion in nanoporous solids with molecular dynamics and transition state theory (umbrella sampling).
 - Study, design and simulation of new MOF structures with various design approaches: metal replacement, mixed-metal frameworks, ligand replacement and confinement of ionic liquids. Tailoring of adsorption and separation properties of zeolite and MOF frameworks through structure modification
 - Force field design, development and optimization of new MOF structures.
 - Simulation of temperature response of structure and negative thermal expansion with the use of lattice dynamics methods.
- Big Data Analysis
 - Supervised Machine Learning methods
- Experimental structure determination with use of XRD – powder XRD measurements of zeolites, MOFs/ZIFs:
 - Preparation of sample and measurement
 - Analysis of XRD patterns for the determination of unit cell size: indexing and pattern refinement with Rietveld and Le Bail methods.

SCIENTIFIC SKILLS AND TOOLS

- Programming languages: FORTRAN 90/95, MATLAB, Python, Bash (Linux/OS X)
- Parallel computing and super-computing (experience with PBS and Slurm batch systems)
- Molecular dynamics: GROMACS, LAMPPS, Materials Studio (FORCITE and DISCOVER programs), GULP (General Utility Lattice Program)
- Monte Carlo: CASSANDRA, Materials Studio
- Process modeling: gProms® process modeling platform
- GSAS for the XRD pattern analysis and extraction of unit cell size.
- Use of crystal visualizers and crystal builder programs for unit cell visualization and reconstruction: VMD, Crystal Viewer, Discovery Studio, CrystalMaker, Avogadro, Jmol, Chimera, iRaspa
- Multiplatform experience: Workstations operating in Linux, Windows and MacOS

FURTHER EDUCATION: COURSES, WORKSHOPS, TUTORIALS

Specializations

1. Data Science Professional. Wednesday, October 22, 2021
<https://coursera.org/share/760be1e170f6a137dc3ba243215f5b02>
2. Introduction to Data Science. July 15, 2021
<https://www.coursera.org/account/accomplishments/specialization/certificate/ZRL3HU3S9D8B>

Courses

1. Applied Data Science Capstone. Wednesday, October 22, 2021
<https://coursera.org/share/017f3f93c0594abae8f39c6986915cf5>
2. Machine Learning with Python. Certificate earned at Saturday, July 15, 2021
<https://www.coursera.org/account/accomplishments/certificate/UHPR6TF86TBJ>
3. Databases and SQL for Data Science with Python. Certificate earned at Saturday, June 19, 2021
<https://coursera.org/share/ad73baba9e676a89d2c097b156919391>
4. Python Project for Data Science. Certificate earned at Friday, May 28, 2021
<https://coursera.org/share/23c29bfd114baca5ff09bcdcc450734b>
5. Data Science Methodology. Certificate earned at Thursday, May 27, 2021.
<https://coursera.org/share/4ea0b38131352b78520041658bbcb265>
6. Tools for Data Science. Certificate earned at Tuesday, May 25, 2021
<https://coursera.org/share/9c3c8c1c63ef728e9752b4fdc7611a39>
7. What is Data Science on Coursera. Certificate earned at Wednesday, May 12, 2021
<https://coursera.org/share/22bce52cba2429a102e8457f68de5e38>
8. Data Analysis with Python by IBM on Coursera. Certificate earned at Saturday, November 30, 2019 6:56 AM GMT
(https://www.coursera.org/account/accomplishments/certificate/LEAY64NPPSB6?utm_medium=certificate&utm_source=link&utm_campaign=copybutton_certificate)
9. Python for Data Science and AI by IBM on Coursera. Certificate earned at Thursday, November 7, 2019 7:23 PM GMT
(https://www.coursera.org/account/accomplishments/certificate/3XLFWK5NSCD9?utm_medium=certificate&utm_source=link&utm_campaign=copybutton_certificate)
10. Data Visualization with Python by IBM on Coursera. Certificate earned at Monday, December 16, 2019 1:18 PM GMT
(https://www.coursera.org/account/accomplishments/certificate/ATJS3E34YJF2?utm_medium=certificate&utm_source=link&utm_campaign=copybutton_certificate)
11. Python – Tutorial in Python programming, 29 February 2016, at TAMUQ
12. gPROMS – An Introduction to gPROMS, 14-16 November 2011, at PSEL Head Office, London