

## From atoms and molecules to materials: Design of novel membranes for gas separation

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The unprecedented increase of computing power at affordable price and the development of advanced computational techniques spanning from the sub-molecular all the way to the macroscopic engineering level has made computational molecular engineering a very powerful tool for the design of novel advanced materials with tailor-made properties. In this lecture, we will present a predictive model for the accurate design of highly selective Zeolitic-imidazolate Frameworks (ZIFs) for the separation of various gas mixtures, using a combination of Density Functional Theory (DFT) calculations, molecular simulation (both Molecular Dynamics and Grand Canonical Monte Carlo) and finally a Machine Learning model that allows massive screening of various structures whose relevant properties are generated by molecular simulation or experimental data [1]. Furthermore, a coarse-grained model based on Martini 3 representation will be shown to provide accurate structural and permeability predictions for various gases in ZIFs [2]. This approach can be generalized and used for other nanoporous materials for various applications. An immediate example refers to mixed matrix membranes where ZIFs are dispersed in a polymer matrix. In this application, a coarse-grained model for the polymer based on Martini 3 will be also presented [3]. Model predictions are in excellent agreement with experimental data [4].

### References

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## Ioannis G. Economou



Professor Ioannis G. Economou is Visiting Professor in the Department of Chemical and Biological Engineering of Friedrich-Alexander-Universität Erlangen-Nürnberg. He holds a Diploma in Chemical Engineering from the National Technical University of Athens, Greece (1987) and a PhD also in Chemical Engineering from The Johns Hopkins University in Baltimore, Maryland, USA (1992). He was a post-doctoral researcher in Delft University of Technology in the Netherlands (1993 – 94) and in Exxon Research and Engineering Company, in New Jersey, USA (1994 – 95). From 1995 to 2009, he worked at the National Center for Scientific Research “Demokritos” in Athens, Greece where he held the position of Director of Molecular Thermodynamics and Modeling of Materials Laboratory from 2003 to 2021 (while on leave from 2009 to 2015, and 2016 to 2021). From 2009 until 2012, he was the Associate Provost for Graduate Studies and Professor of Chemical Engineering at the Petroleum Institute, Abu Dhabi. In 2013, he was appointed Professor of Chemical Engineering at Texas A&M University at Qatar (TAMUQ), in 2017 Associate Dean for Academic Affairs, in 2021 Senior Associate Dean for Academic Affairs and Graduate Studies and from July 2023 until July 2024, he was the Executive Associate Dean of TAMUQ. He is a Fellow of the American Institute of Chemical Engineers (2021).

He held various visiting / research positions including research fellow in University College London (1994 – 96 as a Marie Curie Fellow of the European Commission) and Princeton University (2004 and 2015), and visiting Professor in the Technical University of Denmark (2001 and 2006 - 07) and the American College of Greece (2007 - 09). Furthermore, he has consulted extensively for major oil and chemical companies in North America, Europe and Middle East.

Prof. Economou’s research interests are related to the development and validation of molecular and macroscopic thermodynamic models for the oil & gas, chemical and pharmaceutical industry. In recent years, he developed models for CO<sub>2</sub> capture, transportation and sequestration technologies, shale gas technology, aqueous systems, green solvents, pharmaceuticals, and soft materials including organic and inorganic membranes, polymers, ionic liquids, metal organic frameworks, etc. He has been the project director for 30 research projects funded by the European Commission, national funding agencies in Greece and in Qatar, and industry, and principal investigator for another 17 projects. He has raised more than 10 million € of external research funding.

Prof. Economou has supervised 20 MSc students, 15 PhD students and 23 post-docs, he has published 240 peer-reviewed research papers in leading journals in Chemical Engineering, Physical Chemistry and Polymer Science. In addition, he co-authored 10 book chapters and co-edited 1 book entitled “Natural Gas Processing from Midstream to Downstream” (Wiley, 2019). His H-index is 59 according to Scholar Google. He has given approximately 400 presentations in conferences, Universities and industrial research centers worldwide. He has served as external examiner for 25 PhD theses in 11 countries (Europe, Latin America and Middle East). He is Editor of *Fluid Phase Equilibria* (Elsevier).