The Warsaw Doctoral School in Natural and Biomedical Sciences and
the Institute of Physics PAS cordially invites you to a **SPOTLIGHT TALK**

Molecular Simulations: A computational toolbox to predict, understand and rationally tailor the physicochemical properties of liquid and supercritical solvents and materials for sustainable chemical applications

given by

Dr Ioannis Skarmoutsos

Department of Chemistry, University of Ioannina, 45110 Ioannina, Greece

on 24th April 2024, 12:30 at the IP PAS Conference room 203, building I
Duration: 45 min + question time

The event will be available on ZOOM also, at this link

All Warsaw-4-Phd students (and others) very welcome!

Abstract of the talk:

Molecular simulation techniques, following the principles of Classical/Quantum Statistical Mechanics, have become indispensable tools, not only for theoretical chemists and molecular physicists, but also for a wide spectrum of researchers working in a variety of other fields. Molecular simulations have served to obtain values of various physicochemical properties (often inaccessible experimentally), to verify molecular-based theories and to gain insight into the molecular principles underlying various processes. In such a way, their explanatory and predictive capabilities can be extremely helpful for the rational design of solvents and materials with tailored properties for specific applications.
In this lecture, a summary of our research efforts to address fundamental issues related to green and sustainable chemical applications using multi-scale molecular simulation techniques will be discussed. More specifically, our research studies focused on revealing novel aspects on the thermodynamics, structure and dynamics of:

i) Molecular and ionic liquids for energy storage applications
ii) Nanoporous materials for greenhouse gas and water capture and purification.
iii) Supercritical Fluids will be systematically presented. Future perspectives and open problems will also be outlined

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About the speaker:

Dr Ioannis Skarmoutsos is Assistant Professor at the University of Ioannina since 2022. He received his diploma in Chemistry in 2000, and his M.Sc. and Ph.D. in Physical Chemistry in 2003 and 2006, respectively, from the National and Kapodistrian University of Athens. He spent several postdoc years at the Universitat Politècnica de Catalunya (2008-2009), Imperial College London (2009-2011), University of Sassari (20212), University of Crete (2012-2013), CEA Grenoble (2013-2015), University College London (2015-2016), University of Montpellier 2 (2016-2018), and National Hellenic Research Foundation in collaboration with Aristotle University and FORTH/ICE-HT (2019-2022).

He possesses interdisciplinary skills in computational materials science with expertise in first principles and molecular-level calculations. His research has dealt with hydrogen bonding networks and related dynamics in supercritical fluids and liquid aqueous solutions, ionic liquids, adsorption and separation of gas mixtures in carbon-based nanoporous materials, organic electrolytes with applications in battery technology, computational modelling of the plastic phase of water, MOF-based materials for gas storage and separation, and pillared graphene-based porous materials for energy storage applications.