CURRICULUM VITAE

IOANNIS SKARMOUTSOS

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EDUCATION

- Ph.D. in Physical and Theoretical Chemistry, University of Athens, Greece (2006)
- M.Sc. in Physical Chemistry, University of Athens, Greece (2003)
- B.Sc. in Chemistry, University of Athens, Greece (2000)

PROFESSIONAL EXPERIENCE AND APPOINTMENTS

04/2019– present:	Research Associate, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Greece.
01/2019 – 03/2019:	HPC Europa 3 Research Fellow, Universidad Pablo de Olavide, Department of Physical, Chemical, and Natural Systems, Seville, Spain.
10/2016 – 12/2018:	Research Associate, Institut Charles Gerhardt (UMR, CNRS 5253), University of Montpellier 2, Montpellier, France.
04/2015 - 05/2016:	Research Associate. University College London (UCL), Department of Earth Sciences – Department of Physics and Astronomy, London, UK.

10/2013 - 03/2015: Research Engineer (Ingénieur Chercheur), Institute for Nanosciences and Cryogenics, Commissariat à l'énergie atomique et aux énergies alternatives (CEA), Grenoble, France.

09/2012 - 08/2013: Research Associate, Department of Chemistry, University of Crete Heraklion, Greece.

04/2012 - 06/2012: HPC Europa 2 Research Fellow, University of Sassari, Department of Chemistry and Pharmacy, Sassari, Italy.

09/2009 - 09/2011: Research Associate, Imperial College London, Department of Chemistry, London, UK.

04/2008 - 04/2009: Research Fellow, Universitat Politècnica de Catalunya (UPC), Department of Physics and Nuclear Engineering, Barcelona, Spain.

MAIN RESEARCH INTERESTS

- Investigation of the properties of liquid and supercritical solvents for green chemistry applications.
- Thermodynamic, structural and dynamic properties of bulk ionic liquids.
- Computational modelling-rational design of nanoporous materials for the adsorption and separation of gases/liquids for energy and environmental applications.
- Investigation of the properties of organic electrolytes for battery applications.
- Investigation of the properties of water and aqueous solutions.
- Computational modelling of new alternative refrigerants.

GRANTS AWARDED

- Universitat Politecnica de Catalunya (UPC), Research Fellowship, Project: "Theoretical-computational investigation of the structural and dynamic properties of molecular systems in condensed phases via computer simulations.", Department of Physics and Nuclear Engineering, 2008.

TEACHING EXPERIENCE

- Laboratory of Computational Chemistry, Department of Chemistry, Imperial College London, UK, 2009-2010.

- Seminar Series in "Statistical Mechanics and Molecular Simulation Methods" for postgraduate students, Department of Physics and Nuclear Engineering, SIMCON, Universitat Politecnica de Catalunya, Spain 2008-2009.
- Laboratory of Physical Chemistry, Department of Chemistry - Department of Pharmacy, University of Athens, Greece, 2000-2002.

PROFESSIONAL AFFILIATIONS & ACTIVITIES

- Member of the Association of Greek Chemists (EEX).
- Member of the European Molecular Liquids Group (EMLG).
- Member of the editorial board of the Journal of Theoretical Chemistry (Hindawi Publishing Corporation) (2012-2017).
- Reviewer for 21 international peer-reviewed scientific journals in the fields of physical chemistry, chemical physics, chemical engineering, materials science, energy and environmental applications and molecular modelling.
- Scientific Project Evaluator for granting access to the High Performance Computing facilities of the Greek Research and Technology Network (GRNET).

AWARDS AND DISTINCTIONS

- HPC – Europa 3 project: "Ab Initio Molecular Dynamics of Mixtures of Ionic Liquids with Organic Carbonate Electrolytes ". Project awarded by the European Union (2018). Role: Principal Investigator. (host: Prof. Sofia Calero, Universidad Pablo de Olavide, Seville, Spain)
- "A joint experimental and theoretical study of supercritical mixtures." Project awarded by the Science and Technology Facilities Council (STFC), United Kingdom (UK) (2016). Role: Co-Investigator (PI: Dr Sarantos Marinakis, Queen Mary University of London, Co-Investigator: Prof. Alan Soper, STFC).
- "FPMDCISTRANS: First Principles Molecular Dynamics studies of Cis- and Trans-N-Methylformamide liquid mixtures." Project Awarded by the Greek Research and Technology Network (GRNET) (2016). Role: Principal Investigator (together with Prof. Jannis Samios, University of Athens).
- HPC – Europa 2 project to study the properties of water and aqueous solutions using ab initio molecular dynamics simulations. Project awarded by the European Union (2012). Role: Principal Investigator (host: Dr Marco Masia, University of Sassari, Italy).

SELECTED PUBLICATIONS

1. I. Skarmoutsos, G. Maurin, E. Guardia, J. Samios, "Hydration structure and dynamics of the favipiravir antiviral drug: A molecular modelling approach.", *Bull. Chem. Soc. Jpn.* 2020, https://doi.org/10.1246/bcsj.20200163
2. I. Skarmoutsos, E. N. Koukaras, C. Galiotis, G. Froudakis, E. Klontzas, "Porous carbon nanotube networks and pillared graphene materials exhibiting high SF_6 adsorption uptake and separation selectivity of SF_6/N_2 fluid mixtures: A comparative molecular simulation study.", *Micropor. Mesopor. Mat.* 2020, 307, 110464.
3. I. Skarmoutsos, E. Guardia, "Solvation Structure and Dynamics of the Dimethylammonium Cation Diluted in Liquid Water: A Molecular Dynamics Approach.", *J. Chem. Phys.* 2020, 152, 234501.
4. I. Skarmoutsos, M. Eddaoudi, G. Maurin, "Highly efficient rare-earth based metal–organic frameworks for water adsorption: A molecular modelling approach.", *J. Phys. Chem. C* 2019, 123, 26989.
5. I. Skarmoutsos, L. Spyrogiannopoulos, E. Kainourgiakis, J. Samios, "On the interplay between the local structure and dynamics in low concentration mixtures of H_2O and HOD in the $[Emim^+][TF2N^-]$ room temperature ionic liquid.", *J. Mol. Liq.* 2019, 289, 111135.
6. I. Skarmoutsos, S. Mossa, E. Guardia, "The effect of polymorphism on the structural, dynamic and dielectric properties of plastic crystal water: A molecular dynamics simulation perspective.", *J. Chem. Phys.* 2019, 150, 124506.
7. I. Skarmoutsos, E. Guardia, J. Samios, "Local structural fluctuations, hydrogen bonding and structural transitions in supercritical water.", J. Supercrit. Fluids 2017, 130, 156.
8. M. B. Jiang, V. Ponnuchamy, Y. Shen, X. Yang, K. Yuan, V. Vetere, S. Mossa, I. Skarmoutsos, Y. Zhang, J. Zheng, "The Anion Effect on Li^+ Ion Coordination Structure in Ethylene Carbonate Solutions.", *J. Phys. Chem. Lett.* 2016, 7, 3554.
9. I. Skarmoutsos, V. Ponnuchamy, V. Vetere, S. Mossa, "Li^+ solvation in pure, binary and ternary mixtures of organic carbonate electrolytes.", *J. Phys. Chem. C* 2015 119, 4502.
10. E. Guardia, I. Skarmoutsos, M. Masia, "Hydrogen bonding and related

properties in liquid water: A Car-Parrinello molecular dynamics simulation study.", *J. Phys. Chem. B* 2015, 119, 8926.

11. I. Skarmoutsos, T. Welton, P. A. Hunt, "The Importance of Timescale for Hydrogen Bonding in Imidazolium Chloride Ionic Liquids.", *Phys. Chem. Chem. Phys.* 2014, 16, 3675.
12. I. Skarmoutsos, D. Dellis, R. P. Matthews, T. Welton, P. A. Hunt, "Hydrogen Bonding in 1-Butyl- and 1-Ethyl-3-Methylimidazolium Chloride Ionic Liquids J. Phys. Chem. B, 116, 4921 (2012).", *J. Phys. Chem. B* 2012, 116, 4921.
13. I. Skarmoutsos, P. A. Hunt, "Structural and dynamic properties of the new alternative refrigerant 2,3,3,3-Tetrafluoro-1-propene (HFO-1234yf) in the liquid state", *J. Phys. Chem. B* 2010, 114, 17120.
14. E. Guardia, I. Skarmoutsos, M. Masia "On ion and molecular polarization of halides in water.", *J. Chem. Theory Comput.* 2009, 5, 1449.
15. I. Skarmoutsos, D. Dellis, J. Samios, "The effect of intermolecular interactions on local density inhomogeneities and related properties in pure supercritical molecular fluids. A comparative molecular dynamics study.", *J. Phys. Chem. B* 2009, 113, 2783.