

CURRICULUM VITAE

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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 SF₆ adsorption uptake and separation selectivity of SF₆/N₂ 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 H₂O 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.](#)