Dr IOANNIS SKARMOUTSOS

Born in Vasilika Fthiotidas, Greece

28 March 1977

Nationality: Greek

iskarmoutsos@hotmail.com

ACADEMIC EDUCATION

2003-2006 **Ph. D. in Physical Chemistry,** National and Kapodistrian **University of Athens.**
Department of Chemistry, Physical Chemistry Laboratory, Supervisor: Prof. Jannis Samios
"Theoretical-Computational investigation of the influence of thermodynamic parameters on the macroscopic, structural and dynamic properties of supercritical molecular systems".

2003 **M.Sc. in Physical Chemistry,** National and Kapodistrian **University of Athens**.
Department of Chemistry, Physical Chemistry Laboratory, Supervisor: Dr. Jannis Samios
"A statistical mechanical investigation of the properties of supercritical carbon dioxide and of the liquid mixture cis-trans N-Methylformamide via MD simulation techniques."

2000 **Diploma in Chemistry,** National and Kapodistrian University of Athens, Dpt of Chemistry.
Catalytic reactions with transition metal complexes in aqueous solutions."
Scientific Advisor: Dr George Papadogiannakis (Laboratory of Industrial Chemistry)

WORKING EXPERIENCE

April 2019-	**National Hellenic Research Foundation (NHRF) (In Collaboration with the Aristotle University of Thessaloniki (AUTH) and FORTH/ICE-HT)** **Duties:** *Computational modeling of pillared graphene-based porous materials for energy storage applications*
January 2019- March 2019	**HPC-Europa 3 Research Fellow, Universidad Pablo de Olavide, Seville, Spain** **Duties:** *i) Computational modeling of mixtures of ionic liquids with organic battery electrolytes ii) MOF-based materials for the removal of organic contaminants from water.*
October 2016- December 2018	**Research Associate**, **Institut Charles Gerhardt (UMR, CNRS 5253), University of Montpellier 2, Montpellier, France** **Duties:** *Computational modeling of MOF-based materials for gas storage and separation.*
June 2016- July 2016	**Visiting Researcher**, **Universitat Politècnica de Catalunya (UPC), Spain.** Department of Physics **Duties:** *Computational modeling of the plastic phase of water.*
May 2016- June 2016	**Visiting Researcher**, **University of Athens, Greece** Department of Chemistry – Laboratory of Physical Chemistry **Duties:** *Computational modeling of liquids at elevated pressures.*

Apr. 2015- May 2016	**Research Associate**. **University College London (UCL), London, UK.** Department of Earth Sciences – Department of Physics and Astronomy **Funding:** ERC European project **Duties:** *Computational modeling of aqueous systems using ab initio molecular dynamics simulations.*
Oct. 2013- March 2015	**Research Engineer** (Ingénieur Chercheur). **CEA, Grenoble, France.** Institute for Nanoscience and Cryogenics (INAC-SPrAM) **Funding:** ANR ALIBABA project **Duties:** *Computational modeling of organic electrolytes with applications in battery technology.*
Sept.2012 – August 2013	**Research Associate** position at **University of Crete, Greece**. Materials Modeling & Design Group, Department of Chemistry **Funding:** THALES Research Project **Duties:** *Computational modeling of adsorption and separation of gas mixtures in carbon-based nanoporous materials.*
Apr.2012 – June 2012	**HPC-Europa 2 Research Fellow. Univ. of Sassari, Italy**. **Funding:** HPC-Europa European Union fellowship **Duties:** *To use the High Performance Computing facilities of the supercomputing center of CINECA to study the behavior of water and aqueous solutions by means of ab initio molecular dynamics simulations.*
Sept.2009 – Sept 2011	**Research Associate**, **Imperial College, London, UK** Dept. of Chemistry, Webpage: http://www.huntresearchgroup.org.uk **Funding:** ERC European Project. **Duties:** *To employ computational techniques like molecular simulation and ab initio quantum chemical calculations to investigate the thermodynamical, structural and dynamic properties of ionic liquids.*
Apr.2008 – Apr. 2009	**Post-Doctoral** research fellow, **Univ. Politècnica de Catalunya (UPC), Spain.** *Computer Simulation in Cond. Matt. Res. Group*, http://simcon.upc.edu/people **Funding:** Fellowship of the UPC **Duties:** *to employ molecular dynamics simulation techniques to investigate local structural effects,characteristics of hydrogen bonding networks and related dynamics in supercritical fluids.*

SCIENTIFIC ACHIEVEMENTS

- **39 Publications** in International Peer-Reviewed Journals (See Appendix)

- **2** Papers Submitted for publication in International Peer-Reviewed Journals
- **5** Papers in preparation for submission in International Peer-Reviewed Journals
- **910** Citations (Source: Google Scholar)
- **h-index: 18** (source: Google Scholar)
- **i10-index: 24** (Source: Google Scholar)
- **1** publication in a scientific book (see Appendix)
- **4** Papers in conference proceedings (see Appendix)
- **2** Republished papers (see Appendix)
- **16** Invited Lectures (see Appendix)
- **16** Poster Presentations (see Appendix)
- **13** Talks in conferences (See Appendix)
- **4** Awarded scientific projects
- **1** Awarded Research Fellowship

AWARDED SCIENTIFIC PROJECTS

1. **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).

   Principal Investigator: Dr Ioannis Skarmoutsos

   Co-Investigator: Dr Marco Masia, University of Sassari, Department of Chemistry and Pharmacy.

2. **A joint experimental and theoretical study of supercritical mixtures.**

   Project awarded by the Science and Technology Facilities Council (STFC), United Kingdom (UK) (2016).

   Principal Investigator: Dr Sarantos Marinakis, Queen Mary University of London

   Co-Investigator: Dr Ioannis Skarmoutsos

   Co-Investigator: Professor Alan K. Soper, Science and Technology Facilities Council, UK

3. **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).

   Principal Investigator: Dr Ioannis Skarmoutsos

   Principal Investigator: Professor Jannis Samios, University of Athens, Greece, Department of Chemistry, Director of Laboratory of Physical Chemistry

4. **HPC – Europa 3 project:** "Ab Initio Molecular Dynamics of Mixtures of Ionic Liquids with Organic Carbonate Electrolytes ". Project awarded by the European Union (2018).

   Principal Investigator: Dr Ioannis Skarmoutsos

   Co-Investigator: Professor Sofia Calero, Universidad Pablo de Olavide, Sevilla, Spain, Department of Physical, Chemical and Natural Systems.

SCIENTIFIC TRAINING

2016 Annual CP2K-UK Users Meeting, *United Kingdom*	Third annual CP2K-UK users meeting organized by University College London, Kings College London and EPCC (EPSRC funded).
2013 Summer School *Italy*	International School of Physics "Enrico Fermi": Water: Fundamental as a basis for understanding the environment and promoting technology.
2012 GPU workshop *Cyprus Institute*	Organized by the Computation-based Science and Tech. Research Centre (CaSToRC), in the framework of LinkSCEEM-2 and Cy-Tera projects.
2005 Summer School *Cardiff University- UK.*	CCP5 and Marie Curie Actions: Methods in Molecular Simulation Summer School, Advanced Courses in " *First Principles Simulations"*
2002 Winter School *Germany-Netherlands*	Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms, John von Neumann Institute for Computing (NIC)
2002 Summer School *Greece*	NATO Advanced Study Institute (ASI): Novel Approaches to the Structure and Dynamics of Liquids: Experiments, Theories and Simulations.

COMPUTING SKILLS

Programming	Fortran 77/90, experience in Unix systems, Linux, Mac OS, Windows.
Computing	**Use of High Performance Computing Systems** (HPC Imperial College, Grace-UCL, Mare Nostrum BSC Barcelona, CINECA, Julich Germany, Titan-USA)
MD packages	**Extensive knowledge of molecular simulation** packages DL_POLY, Moscito, Moldy, Moliq-Dynamo and working experience with the ab initio codes CPMD, CP2k, Gaussian, GaussView and Materials Studio.
MC packages	Very good working experience with the Monte-Carlo codes RASPA and CADSS.
Theoretical Chemistry Development	**Development of utility software**, for analysis of molecular trajectories of MD simulations (constructed for the Moscito, Moldy, DL_POLY, cp2k and CPMD, RASPA codes), to investigate structural and dynamic properties of fluid molecular systems.

AWARDED RESEARCH FELLOWSHIPS

• 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 AND OTHER SCIENTIFIC ACTIVITIES

Teaching in pre-graduate students (Chemistry-Pharmacy), Lab. of Phys. Chemistry, Athens (**3 semesters**).
Teaching in pre-graduate students (Chemistry), Theoretical Chemistry Laboratory (Imperial College London, UK) (**2 semesters**), Teaching of application of Informatics in Chemistry in pre-graduate students, Department of Chemistry, University of Athens (**2 semesters**), Teaching of statistical mechanics and molecular simulation techniques in post-graduate students, Department of Physics, Technical University of Catalonia (**2 semesters**)

Reviewer for 24 international scientific journals: *Journal of Physical Chemistry, Chemical Physics Letters, Chemical Physics, Physical Chemistry Chemical Physics, Fuel, Journal of the Brazilian Chemical Society, Journal of Molecular Liquids, International Journal of Modern Physics B, International Journal of Heat and Mass Transfer, Microporous and Mesoporous Materials, Advanced Theory and Simulations, Journal of Molecular Graphics and Modelling, New Journal of Chemistry, ACS Energy Letters, Fluid Phase Equilibria, Journal of Industrial and Engineering Chemistry, Journal of Photochemistry and Photobiology A: Chemistry, Journal of Chemical Information and Modeling, Chinese Physics B, Entropy, Applied Surface Science, Journal of Inorganic and Organometallic Polymers and Materials, Applied Thermal Engineering, Journal of CO_2 Utilization*
Reviewer for the Greek Research & Technology Network (GRNET) High Performance Computing Services
Member of the *European Molecular Liquids Group* (EMLG) (http://139.30.122.11/EMLG/index.html).
Member of the editorial board of the *Journal of Theoretical Chemistry* (Hindawi Publishing Corporation) from 28-11-2012 to 23-07-2017.
Member of the editorial board of *Frontiers in Physics, Condensed Matter Physics* (Frontiers Media, Lausanne, Switzerland) from 07-11-2020.

LANGUAGES

Greek (native), English (fluent, working experience), Spanish (very good knowledge, working experience), French (higher intermediate level, working experience)

REFERENCES

References may be asked from the following academics:

Dr Stefano Mossa
INAC/SPrAM (UMR 5819 UJF, CNRS, CEA), CEA-Grenoble, 17 Rue des Martyrs, 38054 Grenoble, France
Email: stefano.mossa@cea.fr

Prof. George E. Froudakis
Department of Chemistry, University of Crete, Voutes, Heraklion, 71003 Crete, Greece
Email: frudakis@chemistry.uoc.gr

Dr Patricia Hunt
Department of Chemistry, Exhibition Rd, Imperial College of Science, Technology and Medicine, South Kensington, London, SW7 2AZ , United Kingdom
Email: p.hunt@imperial.ac.uk
Web page : http://www.huntresearchgroup.org.uk/index.html

Prof. Tom Welton
Dean of the Faculty of Natural Sciences, Imperial College of Science, Technology and Medicine, Exhibition Rd, South Kensington, London, SW7 2AZ , United Kingdom
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Prof. Elvira Guardia
Departament de Física i Enginyeria Nuclear, Universitat Politècnica de Catalunya, Edifici B4-B5, Campus Nord, Jordi Girona 1-3, 08034 Barcelona, Spain
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Dr Marco Masia
Dipartimento di Chimica, Università degli studi di Sassari, Via Vienna 2, 07100, Sassari, Italy
Email: marco.masia@uniss.it
Web page : http://physchem.uniss.it/marco.masia/about.html

Prof. Jannis Samios
National & Kapodistrian University of Athens, Department of Chemistry, Physical Chemistry Laboratory, Panepistimiopolis 15771, Athens , Greece
Email: isamios@chem.uoa.gr

Prof. Guillaume Maurin
Institut Charles Gerhardt (UMR, CNRS 5253), University of Montpellier 2, Montpellier, France
Email: guillaume.maurin@univ-montp2.fr

APPENDIX

Publications in International Journals with referees

1) **Confinement effects on the properties of polar hydrogen-bonded fluids: A showcase on methanol adsorbed in three-dimensional pillared graphene and carbon nanotube networks.**

Ioannis Skarmoutsos, Emmanuel N. Koukaras, George E. Froudakis, Guillaume Maurin and Emmanuel Klontzas, *J. Phys. Chem. C* **124**, 22959 (2020)

2) **Hydration structure and dynamics of the favipiravir antiviral drug: A molecular modelling approach.**

Ioannis Skarmoutsos, Guillaume Maurin, Elvira Guardia and Jannis Samios, *Bull. Chem. Soc. Jpn*. **93**, 1378 (2020)

3) **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.**

Ioannis Skarmoutsos, Emmanuel N. Koukaras, Costas Galiotis, George Froudakis, Emmanuel Klontzas *Micropor. Mesopor. Mat.* **307**, 110464 (2020)

4) **Solvation Structure and Dynamics of the Dimethylammonium Cation Diluted in Liquid Water: A Molecular Dynamics Approach**

Ioannis Skarmoutsos and Elvira Guardia *J. Chem. Phys.* **152**, 234501 (2020)

5) **Highly efficient rare-earth based metal–organic frameworks for water adsorption: A molecular modelling approach.**

Ioannis Skarmoutsos, Mohamed Eddaoudi and Guillaume Maurin (2019) *J. Phys. Chem. C* **123**, 26989 (2019)

6) **A study of Ar-N_2 supercritical mixtures using neutron scattering, molecular dynamics simulations and quantum mechanical scattering calculations.**

Alan K. Soper, Ioannis Skarmoutsos, Jacek Klos, Jannis Samios and Sarantos Marinakis (2019) *J. Mol. Liq.* **290**, 111168 (2019)

7) **On the interplay between the local structure and dynamics in low concentration mixtures of H_2O and HOD in the [$Emim^+$][TF_2N^-] room temperature ionic liquid.**

Ioannis Skarmoutsos, Leonidas Spyrogiannopoulos, Emmanouil Kainourgiakis and Jannis Samios *J. Mol. Liq.* **289**, 111135 (2019)

8) **The effect of polymorphism on the structural, dynamic and dielectric properties of plastic crystal water: A molecular dynamics simulation perspective.**

Ioannis Skarmoutsos, Stefano Mossa and Elvira Guardia (2019) *J. Chem. Phys.* **150**, 124506 (2019)

9) **Highly tunable sulfur hexafluoride separation by interpenetration control in metal organic frameworks.**

Ioannis Skarmoutsos, Mohamed Eddaoudi and Guillaume Maurin, *Micropor. Mesopor. Mat.* **281**, 44 (2019)

10) **Solvent and Salt Effect on Lithium Ion Solvation and Contact Ion Pair Formation in Organic Carbonates: A Quantum Chemical Perspective.**

Veerapandian Ponnuchamy, Stefano Mossa and Ioannis Skarmoutsos *J. Phys. Chem. C* **122**, 25930 (2018)

11) **Peculiar Molecular Shape and Size Dependence of the Dynamics of Fluids confined in a Small-Pore Metal-Organic Framework.**

Ioannis Skarmoutsos, Mohamed Eddaoudi and Guillaume Maurin, *J. Phys. Chem. Lett.* **9**, 3014 (2018)

12) **CO_2 capture using the SIFSIX-2-Cu-i metal-organic framework: A computational approach.**

Ioannis Skarmoutsos, Youssef Belmabkhout, Karim Adil, Mohamed Eddaoudi and Guillaume Maurin, *J. Phys. Chem. C*, **121**, 27462 (2017)

13) **Local structural fluctuations, hydrogen bonding and structural transitions in supercritical water.**

Ioannis Skarmoutsos, Elvira Guardia and Jannis Samios, *J. Supercrit. Fluids* **130**, 156 (2017)

14) **Local Structure and Translational Dynamics of NMF (N-Methylformamide)– DMF (N, N-Dimethylformamide) Mixtures via Molecular Dynamics Simulation.**

Nikolaos Elpidoforou, Ioannis Skarmoutsos, Emmanuel Kainourgiakis, Vasilios Raptis and Jannis Samios, *J. Mol. Liq.*, **226**, 16 (2017)

15) **Structure and dynamics of liquid CS_2: Going from ambient to elevated pressure conditions.**

Ioannis Skarmoutsos, Stefano Mossa and Jannis Samios, *J. Chem. Phys.*, **145**, 154505 (2016)

16) **The Anion Effect on Li+ Ion Coordination Structure in Ethylene Carbonate Solutions**

Bo Jiang, Veerapandian Ponnuchamy, Yuneng Shen, Xueming Yang, Kaijun Yuan, Valentina Vetere, Stefano Mossa, Ioannis Skarmoutsos, Yufan Zhang and Junrong Zheng, *J. Phys. Chem. Lett.*, **7**, 3554 (2016)

17) **Highly selective separation and adsorption-induced phase transition of SF_6-N_2 fluid mixtures in three-dimensional carbon nanotube networks.**

Ioannis Skarmoutsos, George Tamiolakis and George E. Froudakis *J. Supercrit. Fluids* **113**, 89 (2016)

18) **Structural and dipolar fluctuations in liquid water: A Car-Parrinello molecular dynamics study.**

Ioannis Skarmoutsos, Elvira Guardia and Marco Masia *Chem. Phys. Lett.*, **648**, 102 (2016)

19) **Li^+ solvation in pure, binary and ternary mixtures of organic carbonate electrolytes.**

Ioannis Skarmoutsos, Veerapandian Ponnuchamy, Valentina Vetere and Stefano Mossa *J. Phys. Chem. C*, **119**, 4502 (2015)

20) **Hydrogen bonding and related properties in liquid water: A Car-Parrinello molecular dynamics simulation study.**

Elvira Guardia, Ioannis Skarmoutsos and Marco Masia *J. Phys. Chem. B*, **119**, 8926 (2015)

21) **The Importance of Timescale for Hydrogen Bonding in Imidazolium Chloride Ionic Liquids.**

Ioannis Skarmoutsos, Tom Welton and Patricia A. Hunt *Phys. Chem. Chem. Phys.*, **16**, 3675 (2014)

22) **Separation of CO_2 / N_2 mixtures in 3D carbon-based porous nanotube networks: A molecular dynamics investigation.**

Ioannis Skarmoutsos, George Tamiolakis and George E. Froudakis, *Phys. Chem. Chem. Phys.*, **16**, 876 (2014)

23) **Carbon-based nanoporous networks as media for the separation of CO_2/CH_4 mixtures: A molecular dynamics approach.**

Ioannis Skarmoutsos, George Tamiolakis and George E. Froudakis, *J. Phys. Chem. C*, **117**, 19373 (2013)

24) **Hydrogen Bonding in 1-Butyl- and 1-Ethyl-3-Methylimidazolium Chloride Ionic Liquids**

Ioannis Skarmoutsos, Dimitris Dellis, Richard P. Matthews, Tom Welton and Patricia A. Hunt, *J. Phys. Chem. B*, **116**, 4921 (2012)

25) **Solvation structure and Dynamics of cis- and trans- 1,2 Dichloroethene Isomers in Supercritical Carbon Dioxide. A molecular dynamics simulation study.**

Dimitris Dellis, Ioannis Skarmoutsos and Jannis Samios, *J. Phys. Chem. B*, **115**, 12098 (2011)

26) **Structural and dynamic properties of the new alternative refrigerant 2,3,3,3-Tetrafluoro-1-propene (HFO-1234yf) in the liquid state.**

Ioannis Skarmoutsos and Patricia A. Hunt, *J. Phys. Chem. B*, **114**, 17120 (2010)

27) **Hydrogen bond, electron donor acceptor dimer and residence dynamics in supercritical CO_2-ethanol mixtures and the effect of hydrogen bonding on single reorientational and translational dynamics. A molecular dynamics simulation study.**

Ioannis Skarmoutsos, Elvira Guardia and Jannis Samios, *J. Chem. Phys.*, **133,** 014504 (2010)

28) **Effect of the local hydrogen bonding network on the reorientational and translational dynamics in supercritical water.**

Ioannis Skarmoutsos and Elvira Guardia, *J. Chem. Phys.,* **132** , 074502 (2010)

29) **Molecular simulations of benzene and hexafluorobenzene using new optimized effective potential models: Investigation of the liquid, vapor-liquid coexistence and supercritical fluid phases.**

Dimitris Dellis, Ioannis Skarmoutsos and Jannis Samios, *J. Mol. Liq.,* **153**, 25 (2010)

30) **On ion and molecular polarization of halides in water.**

Elvira Guardia, Ioannis Skarmoutsos and Marco Masia, *J. Chem. Theory Comput.,* **5**, 1449 (2009)

31) **Local structural effects and related dynamics in supercritical ethanol. 2. Hydrogen bonding network and its effect on single reorientational dynamics.**

Ioannis Skarmoutsos and Elvira Guardia, *J. Phys. Chem. B*, **113**, 8898 (2009)

32) **Local structural effects and related dynamics in supercritical ethanol. 1. Mechanisms of local density reorganization and residence dynamics.**

Ioannis Skarmoutsos and Elvira Guardia, *J. Phys. Chem. B*, **113**, 8887 (2009)

33) **The effect of intermolecular interactions on local density inhomogeneities and related properties in pure supercritical molecular fluids. A comparative molecular dynamics study.**

Ioannis Skarmoutsos, Dimitris Dellis and Jannis Samios, *J. Phys. Chem. B*, **113**, 2783 (2009)

34) **Investigation of the local composition enhancement and related dynamics in supercritical CO_2-cosolvent mixtures via computer simulation. The case of ethanol in CO_2.**

Ioannis Skarmoutsos, Dimitris Dellis and Jannis Samios, *J. Chem. Phys.,* **126** , 224503 (2007)

35) **Local Density Augmentation and Dynamic Properties of Hydrogen- and non Hydrogen- Bonded Supercritical Fluids: A Molecular Dynamics Study**

Ioannis Skarmoutsos and Jannis Samios, *J. Chem. Phys.*, **126** , 044503 (2007)

36) **Local Density Inhomogeneities and Dynamics in Supercritical Water: A molecular dynamics simulation approach.**

Ioannis Skarmoutsos and Jannis Samios, *J. Phys. Chem. B*, **110**, 21931 (2006)

37) **Local intermolecular structure and dynamics in binary supercritical solutions. A molecular dynamics simulation study of methane in carbon dioxide.**

Ioannis Skarmoutsos and Jannis Samios, *J. Mol. Liq.,* **125**, 181-186 (2006)

38) **Investigation of the vapor-liquid equilibrium and supercritical phase of pure methane via computer simulations.**

Ioannis Skarmoutsos, Leonidas I. Kampanakis and Jannis Samios, *J. Mol. Liq.*, **117**, 33-41 (2005)

39) **Molecular dynamics of cis/trans N-methylformamide (NMF) liquid mixture using an all atom optimized rigid force field**

Ioannis Skarmoutsos and Jannis Samios, *Chem. Phys. Lett*, **384**, 108-113 (2004)

Papers submitted for publication in International Journals with referees

1) **Pressure-induced structural transitions in supercritical water: From a gas-like fluid to a plastic crystal polymorph.**

Ioannis Skarmoutsos, Elvira Guardia and Jannis Samios (2021)

2) **The impact of ionic liquid loading in carbon nanoporous materials on the separation of CO_2 / CH_4 fluid mixtures: Insights from molecular simulations.**

Ioannis Skarmoutsos, Emmanuel N. Koukaras and Emmanuel Klontzas (2021)

Papers in the final stage before submission for publication in International Journals with referees

1) **Using microscopic structural descriptors to reveal the heterogeneous local translational-orientational order in liquid water: A Car-Parrinello molecular dynamics study.**

Ioannis Skarmoutsos, Giancarlo Franzese and Elvira Guardia

2) **The polar co-solvent effect on caffeine solvation in supercritical CO_2-ethanol mixtures: A molecular modelling approach.**

Ioannis Skarmoutsos, Ioannis D. Petsalakis and Jannis Samios

Republished Papers:

1) **Local Density Augmentation and Dynamic Properties of Hydrogen- and non Hydrogen- Bonded Supercritical Fluids: A Molecular Dynamics Study**

Ioannis Skarmoutsos and Jannis Samios, **republished in the** *Virtual Journal of Biological Physics Research,* **13 (Issue 3)** (2007)

2) **Investigation of the local composition enhancement and related dynamics in supercritical CO_2-cosolvent mixtures via computer simulation. The case of ethanol in CO_2.**

Ioannis Skarmoutsos Dimitris Dellis and Jannis Samios, **republished in the** *Virtual Journal of Biological Physics Research,* **13** (**Issue 12)** (2007)

Publications in Scientific Books:

1) **Molecular Dynamics Simulation of cis-trans N-Methylformamide (NMF) liquid mixture. Structure and Dynamics**.

Ioannis Skarmoutsos and Jannis Samios, *Lecture Series on Computer and Computational Sciences* (VSP International), **1**, 479 (2004)

Papers in Conference Proceedings:

1) **Molecular Dynamics simulation studies of supercritical carbon dioxide using available potential models. Investigation of the bulk thermodynamical, transport and dynamical properties.**

Ioannis Skarmoutsos and Jannis Samios, Winter School: Quantum Simulations of Complex Many-Body Systems: From Theory to Algorithms, *Publication Series of the John von Neumann Institute for Computing (NIC Series),* **Vol. 11**, 20, (2002)

2) **Molecular dynamics studies of cis/trans N-methylformamide (NMF) liquid mixture using a new optimized all atom force field.**

Ioannis Skarmoutsos and Jannis Samios, NATO Advanced Study Institute (ASI): *Novel Approaches to the Structure and Dynamics of Liquids: Experiments, Theories and Simulations.* page 151 (2002)

3) **Investigation of the Local Density Inhomogeneities and Dynamics in Neat Supercritical Fluids using MD simulation techniques: Comparison between Hydrogen- and Non Hydrogen-Bonded fluids.**

Ioannis Skarmoutsos Nikolaos Elpidoforou and Jannis Samios, Winter School: *Computational Nanoscience: Do It Yourself, Publication Series of the John von Neumann Institute for Computing (NIC Series),* page 11, (2006)

4) **Computational Modelling of Nanoporous Materials for Sustainable Energy and Environmental Applications.**

Ioannis Skarmoutsos, Emmanuel Klontzas, Emmanuel N. Koukaras and Guillaume Maurin, Conference Proccedings, *12th Panhellenic Conference of Chemical Engineering (2019).*

PRESENTATIONS

INVITED LECTURES

1) **Molecular modelling and simulation methods to predict and understand the properties of condensed matter: A physicochemical approach to develop modern chemical, environmental and engineering applications**

Ioannis Skarmoutsos, Invited Lecture at the Chemistry Department, University of Ioannina, Greece (2020)

2) **Understanding the properties of aqueous systems and their interactions with nanoporous materials and sustainable ionic liquid solvents to develop environmental, energy storage and geological applications: A computational modelling perspective.**

Ioannis Skarmoutsos, Invited Lecture at the National Hellenic Research Foundation, Athens, Greece (2019).

3) **Computational Modeling of liquid electrolytes and porous materials for sustainable energy applications.**

Ioannis Skarmoutsos, Invited Lecture at the Department of Physical, Chemical, and Natural Systems, Universidad Pablo de Olavide, Seville, Spain (2019).

4) **Computational modeling of modern electrolytes for energy applications**

Ioannis Skarmoutsos, Invited Lecture at the Department of Chemistry of the École Normale Supérieure de Lyon, France (2018).

5) **Gas adsorption and separation using metal-organic frameworks: A computational approach.**

Ioannis Skarmoutsos, Invited Lecture at the Department of Physics, Technical University of Catalonia (UPC), Spain (2018)

6) **Computational modeling of modern electrolytes for energy applications: Structure and dynamics in ionic liquids and their mixtures with water.**

Ioannis Skarmoutsos, Invited Lecture at the Department of Physics, University of Barcelona (UB), Spain (2018)

7) **Gas adsorption and separation using the SIFSIX-2-Cu-i and SIFSIX-2-Cu metal-organic frameworks: A computational approach.**

Ioannis Skarmoutsos, Invited Lecture at the Physical Chemistry Laboratory, Department of Chemistry, National and Kapodistrian University of Athens, Greece (2018)

8) **Local structural and dipolar fluctuations in liquid water: Insights from ab initio molecular dynamics simulations.**

Ioannis Skarmoutsos, Invited lecture at the University of Barcelona (UB) - Physics Department, Barcelona, Catalonia, Spain (2016)

9) **Local structural and dipolar fluctuations in liquid water: Insights from ab initio molecular dynamics simulations.**

Ioannis Skarmoutsos, Invited lecture at the Institut Laue-Langevin (ILL), Grenoble, France (2016)

10) **Hydrogen Bonding Interactions in Ionic Liquids: Insights from molecular simulation.**

Ioannis Skarmoutsos, Invited lecture at INAC/SPrAM, CEA-Grenoble, France (2013)

11) **Hydrogen Bonding interactions and their effect on the properties of self-associating liquids: Insights from molecular simulations.**

Ioannis Skarmoutsos, Invited lecture at the University of University of Crete, Department of Materials Science and Technology, Iraklio, Greece (2012)

12) **Molecular Dynamics Simulation Techniques: A very useful tool to investigate the properties of condensed matter.**

Ioannis Skarmoutsos, Invited lecture at the University of Crete, Department of Chemistry, Iraklio, Greece (2012)

13) **Hydrogen Bonding interactions and their effect on the properties of self-associating liquids: Insights from molecular simulations.**

Ioannis Skarmoutsos, Invited lecture at the University of Sassari, Department of Chemistry and Pharmacy, Sassari, Italy (2012)

14) **Molecular Dynamics Simulation: A useful tool to investigate the properties of gases confined in nanoporous materials.**

Ioannis Skarmoutsos, Invited lecture at the *European Technical School on Hydrogen and Fuel Cells*, Heraklion, Greece (2012).

15) **Supercritical Fluids: An introduction to the physicochemical properties of a "peculiar" state of matter.**

Ioannis Skarmoutsos, Invited Lecture at the Department of Chemical Engineering, Aristotle University of Thessaloniki, Greece (2011)

16) **Supercritical Fluids: Investigation of local density inhomogeneities and related properties using computer simulations.**

Ioannis Skarmoutsos, Invited lecture at the "Day of the research" of the Department of Physics & Nuclear Engineering (Technical University of Catalonia- UPC), Barcelona, Spain (2009)

TALKS IN CONFERENCES

1) **Understanding the interactions of water with nanoporous materials to develop environmental applications: The case of water adsorption in metal-organic frameworks.**

CECAM Workshop: WaterEurope: Multiscale simulations and coarse-grained models for water and aqueous systems, CECAM Headquarters, EPFL, Lausanne, Switzerland (2019)

2) **Computational Modelling of Nanoporous Materials for Sustainable Energy and Environmental Applications.**

12th Panhellenic Conference of Chemical Engineering, Athens-Greece (2019)

3) **On the Peculiar Molecular Shape and Size Dependence of the Dynamics of Fluids Confined in a Small-Pore Metal-Organic Framework**

Energy Landscapes 2018 Conference (organized by the University of Cambridge), Kalamata, Greece (2018)

4) **Local structural fluctuations, hydrogen bonding and structural transitions in supercritical water.**

WaterSpain 2017 Conference, The Zaragoza Scientific Center for Advanced Modeling (ZCAM), Zaragoza, Spain (2017)

5) **Local structural and dipolar fluctuations in liquid water: Insights from ab initio molecular dynamics simulations.**

European Molecular Liquids Group-EMLG Conference entitled: *"Recent Progresses on the Experimental & Theoretical-Computational Techniques for the Study of Liquids and Supercritical Fluids."* in Crete-Greece (2016)

6) **Computational modeling of battery electrolytes: insights from molecular simulations.**

European Molecular Liquids Group-EMLG Conference entitled: *"Molecular Liquids and Soft Matter: From Fundamentals to Applications."* in Roma Tre University- Italy (2014)

7) **Local Structural Inhomogeneities, Hydrogen Bonding and Tetrahedral Structure in Supercritical Water: Insights from Molecular Simulations.**

International School of Physics "Enrico Fermi", Varenna, Italy (2013)

8) **Local density inhomogeneities and related properties in supercritical fluids. A computer simulation study.**

Ioannis Skarmoutsos, Dimitris Dellis* and Jannis Samios, European Molecular Liquids Group-EMLG Conference entitled: *"Understanding solvation from liquid to supercritical conditions."* in Lisboa- Portugal (2008)

9) **MD Simulation of cis-trans N-Methylformamide (NMF) liquid mixture. Structure and Dynamics.**

Ioannis Skarmoutsos Ricardo L. Mancera and Jannis Samios, *CCP5 and Marie Curie Actions: Methods in Molecular Simulation Summer School* , Cardiff University- UK (2005)

10) **Molecular Dynamics Simulation of cis-trans N-Methylformamide (NMF) liquid mixture. Structure and Dynamics.**

Ioannis Skarmoutsos, Ricardo L. Mancera and Jannis Samios, *International Conference of Computational Methods in Sciences and Engineering (ICCMSE),* organized by the **European Society of Computational Methods in Sciences and Engineering (ESCMSE), Athens-Greece** (2004)

11) **Is the hydrogen-bonding network around the cis and trans N-Methylformamide (NMF) conformers responsible for the observation of different diffusion coefficients? A temperature dependent molecular dynamics approach.**

Ioannis Skarmoutsos, Ricardo L. Mancera and Jannis Samios, European Molecular Liquids Group-EMLG Conference entitled: *"Complex Liquids: Fundamental Properties to Industrial Applications."* in Sheffield Hallam University- UK (2004)

12) **Molecular Dynamics simulations of cis-trans N-Methylformamide liquid mixture. Structure, dynamics and hydrogen bonding analysis.**

Ioannis Skarmoutsos and Jannis Samios, European Molecular Liquids Group-EMLG Conference entitled: *"Molecular Liquids. Routes from Local Order to Large-Scale Cooperativity."* in Castelvecchio Pascoli- Italy (2003)

13) **Molecular dynamics studies of cis/trans N-methylformamide (NMF) liquid mixture using a new optimized all atom force field.**

Ioannis Skarmoutsos and Jannis Samios, NATO Advanced Study Institute (ASI): *Novel Approaches to the Structure and Dynamics of Liquids: Experiments, Theories and Simulations.* Rhodes- Greece (2002)

POSTER PRESENTATIONS

1) **Molecular Dynamics Study of H_2O and HOD dissolved in the Room Temperature Ionic Liquid $Emim^+$ $Tf2N^-$: Dynamical and Structural properties**

Leonidas Spyrogiannopoulos, Emmanouil Kainourgiakis, Ioannis Skarmoutsos and Jannis Samios

Athens Conference of Advances in Chemistry (acac2018), organised on the occasion of the centennial anniversary of the Chemistry Department of the National and Kapodistrian Univeristy of Athens.

2) **Molecular Dynamics Study of low concentrated H_2O and HOD dissolved in the Room Temperature Ionic Liquid $Emim^+$ $Tf2N^-$: Dynamical and Structural properties**

Leonidas Spyrogiannopoulos, Emmanouil Kainourgiakis, Ioannis Skarmoutsos and Jannis Samios

Energy Landscapes 2018 Conference (organized by the University of Cambridge), Kalamata, Greece (2018)

3) **CO_2 capture and separation from methane using the SIFSIX-2-Cu-i metal-organic framework: A computational approach.**

Ioannis Skarmoutsos, Youssef Belmabkhout, Karim Adil, Mohamed Eddaoudi and Guillaume Maurin

11th International Symposium on the Characterization of Porous Solids (COPS-XI), Avignon-France (2017)

4) **Structure and dynamics of liquid CS_2: Going from ambient to elevated pressure conditions.**

Ioannis Skarmoutsos, Stefano Mossa and Jannis Samios

European Molecular Liquids Group-EMLG Conference entitled: *"Recent Progresses on the Experimental & Theoretical-Computational Techniques for the Study of Liquids and Supercritical Fluids."* in Crete-Greece (2016)

5) **Short range order and rotational dynamics in plastic crystal phases of water.**

Andres Henao, Ioannis Skarmoutsos, Luis Carlos Pardo and Elvira Guardia

European Molecular Liquids Group-EMLG Conference entitled: *"Recent Progresses on the Experimental & Theoretical-Computational Techniques for the Study of Liquids and Supercritical Fluids."* in Crete-Greece (2016)

6) **Local Structural Inhomogeneities, Hydrogen Bonding and Local Orientational Structure in Supercritical Water: Insights from Molecular Simulations.**

Ioannis Skarmoutsos, Elvira Guardia and Jannis Samios

European Molecular Liquids Group-EMLG Conference entitled: *"Recent Progresses on the Experimental & Theoretical-Computational Techniques for the Study of Liquids and Supercritical Fluids."* in Crete-Greece (2016)

7) **Carbon-based nanoporous networks as media for the separation of CO_2/CH_4 mixtures: A molecular dynamics approach.**

Ioannis Skarmoutsos, George Tamiolakis and George E. Froudakis

30th Panhellenic Conference on Solid-State Physics and Materials Science, Heraklion, Crete-Greece (2014)

8) **Local Structural Inhomogeneities, Hydrogen Bonding and Tetrahedral Structure in Supercritical Water: Insights from Molecular Simulations.**

International School of Physics “Enrico Fermi”, Varenna, Italy (2013)

9) **Carbon based nanoporous networks as media for the separation of CO_2/CH_4 mixtures: A molecular dynamics approach.**

International School of Physics “Enrico Fermi”, Varenna, Italy (2013)

10) **Solvation properties of alkali and halide ions in water from Car-Parinello molecular dynamics simulations**

Ausias-March Calvo, Marco Masia, Ioannis Skarmoutsos and Elvira Guardia

CPMD meeting 2011: *Extending the limits of Ab Initio Molecular Dynamics Simulations for Chemistry, Materials Science and Biophysics, Barcelona-Spain* (2011)

11) **Investigation of the Local Density Inhomogeneities and Dynamics in Neat Supercritical Fluids using MD simulation techniques: Comparison between Hydrogen- and Non Hydrogen-Bonded fluids.**

Ioannis Skarmoutsos Nikolaos Elpidoforou and Jannis Samios, Winter School: *Computational Nanoscience: Do It Yourself , John von Neumann Institute for Computing (NIC)* Julich-Germany (2006)

12) **Local density inhomogeneities and dynamic properties in supercritical fluids. A MD simulation study of neat sc CO_2 and of the binary mixture CH_4-CO_2.**

Ioannis Skarmoutsos and Jannis Samios, *CCP5 and Marie Curie Actions: Methods in Molecular Simulation Summer School* , Cardiff University- UK (2005)

13) **Is the hydrogen-bonding network around the cis and trans N-Methylformamide (NMF) conformers responsible for the observation of different diffusion coefficients? A temperature dependent molecular dynamics approach.**

Ioannis Skarmoutsos, Ricardo L. Mancera and Jannis Samios, European Molecular Liquids Group-EMLG Conference entitled: *"Complex Liquids: Fundamental Properties to Industrial Applications."* in Sheffield Hallam University- UK (2004)

14) **Molecular Dynamics simulations of cis-trans N-Methylformamide liquid mixture. Structure, dynamics and hydrogen bonding analysis.**

Ioannis Skarmoutsos and Jannis Samios, European Molecular Liquids Group-EMLG Conference entitled: *"Molecular Liquids. Routes from Local Order to Large-Scale Cooperativity."* in Castelvecchio Pascoli- Italy (2003)

15) **Supercritical Methane. Investigation of the bulk thermodynamic, structural and dynamic properties.**

Ioannis Skarmoutsos and Jannis Samios, European Molecular Liquids Group-EMLG Conference entitled: *"Molecular Liquids. Routes from Local Order to Large-Scale Cooperativity."* in Castelvecchio Pascoli- Italy (2003)

16) **Molecular dynamics studies of cis/trans N-methylformamide (NMF) liquid mixture using a new optimized all atom force field.**

Ioannis Skarmoutsos and Jannis Samios, NATO Advanced Study Institute (ASI): *Novel Approaches to the Structure and Dynamics of Liquids: Experiments, Theories and Simulations.* Rhodes- Greece (2002)