DR IOANNIS SKARMOUTSOS

SCIENTIFIC PUBLICATIONS

- **39 Publications** in international peer-reviewed journals
- **1** publication in a scientific book chapter
- **4** publications in books of scientific conference proceedings
- **2** Republished articles

Publications in international peer-reviewed journals

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* (2020) https://doi.org/10.1021/acs.jpcc.0c06289

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*. (2020) https://doi.org/10.1246/bcsj.20200163

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)

Republished Articles:

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 Book Chapters:

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)

Publications in Books of 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).*