Δρ. ΙΩΑΝΝΗΣ ΣΚΑΡΜΟΥΤΣΟΣ

Γεννηθείς στα Βασιλικά Φθιώτιδας, Ελλάδα

Ημερομηνία Γέννησης: 28 Μαρτίου 1977

Υπηκοότητα: Ελληνική

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ΑΚΑΔΗΜΑΪΚΗ ΕΚΠΑΙΔΕΥΣΗ

2003-2006 **Διδακτορικό στη Χημεία,** Εθνικό και Καποδιστριακό Πανεπιστήμιο Αθηνών**.** Τμήμα Χημείας, Εργαστήριο Φυσικοχημείας, Επιβλέπων: Καθ. Ιωάννης Σάμιος *"Θεωρητική-υπολογιστική μελέτη της επίδρασης θερμοδυναμικών παραμέτρων στις μακροσκοπικές, δομικές και δυναμικές ιδιότητες μοριακών συστημάτων στην υπερκρίσιμη κατάσταση".* https://phdtheses.ekt.gr/eadd/handle/10442/20859

2003 **Μεταπτυχιακό στη Φυσικοχημεία,** Εθνικό και Καποδιστριακό Πανεπιστήμιο Αθηνών**.** Τμήμα Χημείας, Εργαστήριο Φυσικοχημείας, Επιβλέπων: Καθ. Ιωάννης Σάμιος *"Στατιστική μηχανική μελέτη των ιδιοτήτων του υπερκρισίμου διοξειδίου του άνθρακα και του υγρού μίγματος cis-trans N-Μεθυλοφορμαμιδίου μέσω τεχνικών μοριακών προσομοιώσεων."*

2000 **Πτυχίο στη Χημεία,** Εθνικό και Καποδιστριακό Πανεπιστήμιο Αθηνών. *Καταλυτικές αντιδράσεις με σύμπλοκα μετάλλων μεταπτώσεως σε υδατικά διαλύματα."* Επιβλέπων: Καθ. Γεώργιος Παπαδογιαννάκης (Εργαστήριο Βιομηχανικής Χημείας)

ΕΡΓΑΣΙΑΚΗ ΕΜΠΕΙΡΙΑ

Απρ. 2022-	**Επίκουρος Καθηγητής (Επί Θητεία), Πανεπιστήμιο Ιωαννίνων, Τμήμα Χημείας** **Γνωστικό Αντικείμενο: Θεωρητική Φυσικοχημεία**
Απρ. 2019- Απρ. 2022	**Ερευνητής, Εθνικό Ίδρυμα Ερευνών - Ινστιτούτο Φυσικής και Θεωρητικής Χημείας, Ίδρυμα Τεχνολογίας Έρευνας (ΙΤΕ/ΙΕΧΜΗ) - Α.Π.Θ. (Τμήμα Χημείας)** **Καθήκοντα:** *Υπολογιστική μοντελοποίηση νανοϋλικών με βάση το γραφένιο για εφαρμογές αποθήκευσης ενέργειας.*
Ιαν. 2019 - Μαρτ. 2019	**HPC-Europa 3 Υποτροφία. Universidad Pablo de Olavide, Seville, Spain**. **Καθήκοντα:** *Υπολογιστική μοντελοποίηση μιγμάτων οργανικών ηλεκτρολυτών με ιοντικά υγρά. Μοντελοποίηση νανοπορωδών υλικών (MOF) για διαχωρισμό υγρών μιγμάτων.*
Οκτώβριος 2016- Δεκ. 2018	**Ερευνητής, Institut Charles Gerhardt (UMR, CNRS 5253), University of Montpellier 2, Montpellier, France** **Καθήκοντα:** *Υπολογιστική μοντελοποίηση νανοπορωδών υλικών (MOF) για αποθήκευση και διαχωρισμό αερίων και υγρών.*

Ιούνιος - Ιούλιος 2016	**Επισκέπτης Ερευνητής, Universitat Politècnica de Catalunya (UPC), Spain.** Department of Physics **Καθήκοντα:** *Υπολογιστική μοντελοποίηση της πλαστικής κρυσταλλικής φάσης του νερού.*
Μάιος - Ιούνιος 2016	**Επισκέπτης Ερευνητής, University of Athens, Greece** Department of Chemistry – Laboratory of Physical Chemistry **Καθήκοντα:** *Υπολογιστική μοντελοποίηση υγρών σε πολύ υψηλές πιέσεις.*
Απρ. 2015- Μάιος 2016	**Ερευνητής. University College London (UCL), London, UK.** Department of Earth Sciences – Department of Physics and Astronomy **Χρηματοδότηση:** ERC European project **Καθήκοντα:** Υπολογιστική *μοντελοποίηση υδατικών συστημάτων μέσω κβαντικών μοριακών δυναμικών προσομοιώσεων.*
Οκτ. 2013- Μάρτιος 2015	**Ερευνητής. CEA, Grenoble, France.** Institute for Nanoscience and Cryogenics (INAC-SPrAM) **Χρηματοδότηση:** ANR ALIBABA project **Καθήκοντα:** *Υπολογιστική μοντελοποίηση οργανικών ηλεκτρολυτών με εφαρμογές στην τεχνολογία μπαταριών.*
Σεπτ. 2012 – Αυγ. 2013	**Ερευνητής. University of Crete, Greece**. Materials Modeling & Design Group, Department of Chemistry **Χρηματοδότηση:** THALES Research Project **Καθήκοντα:** *Υπολογιστική μοντελοποίηση της προσρόφησης και διαχωρισμού αερίων μιγμάτων σε νανοπορώδη υλικά με βάση τον άνθρακα.*
Απρ. 2012 – Ιούνιος 2012	**HPC-Europa 2 Υποτροφία. Univ. of Sassari, Italy**. **Χρηματοδότηση:** HPC-Europa European Union fellowship **Καθήκοντα:** Χρήση Υπερυπολογιστικών συστημάτων του ευρωπαϊκού κέντρου *CINECA για μελέτη ιδιοτήτων του νερού και υδατικών συστημάτων μέσω κβαντικών μοριακών δυναμικών προσομοιώσεων.*
Σεπτ. 2009 – Σεπτ. 2011	**Ερευνητής. Imperial College, London, UK** Dept. of Chemistry, Webpage: http://www.huntresearchgroup.org.uk **Χρηματοδότηση:** ERC European Project. **Καθήκοντα:** *Υπολογιστική μοντελοποίηση ιοντικών υγρών.*
Apr.2008 – Apr. 2009	**Ερευνητική Υποτροφία, Univ. Politècnica de Catalunya (UPC), Spain.** *Computer Simulation in Cond. Matt. Res. Group,* http://simcon.upc.edu/people **Χρηματοδότηση:** Research Fellowship of the UPC **Καθήκοντα:** *Υπολογιστική μελέτη των δεσμών υγρογόνου σε υπερκρίσιμα ρευστά.*

ΥΠΟΧΡΕΩΤΙΚΗ ΣΤΡΑΤΙΩΤΙΚΗ ΘΗΤΕΙΑ

Φεβρουάριος 2007 – Φεβρουάριος 2008 (Σώμα Υλικού Πολέμου)

ΕΠΙΣΤΗΜΟΝΙΚΑ ΕΠΙΤΕΥΓΜΑΤΑ

Google Scholar Profile: https://scholar.google.com/citations?hl=en&user=CRCpodIAAAAJ

Μετρικές κατά την ημερομηνία 29-09-2022
- **47 Δημοσιεύσεις** σε Διεθνή περιοδικά με κριτές (βλ. Υπόμνημα)
- **h-index: 20** (Πηγή: Google Scholar)
- **i10-index: 28** (Πηγή: Google Scholar)
- **1** δημοσίευση σε κεφάλαιο επιστημονικού βιβλίου (βλ. Υπόμνημα)
- **4** Δημοσιεύσεις σε βιβλία πρακτικών συνεδρίων (βλ. Υπόμνημα)
- **2** Αναδημοσιευμένες εργασίες (βλ. Υπόμνημα)
- **17** Διαλέξεις έπειτα από πρόσκληση (βλ. Υπόμνημα)
- **19** Παρουσιάσεις Πόστερ σε συνέδρια (βλ. Υπόμνημα)
- **17** Ομιλίες σε συνέδρια (βλ. Υπόμνημα)
- **4** Εγκεκριμένα Ερευνητικά Προγράμματα
- **1** Εγκεκριμένη Διεθνής Ερευνητική Υποτροφία

ΕΓΚΕΚΡΙΜΕΝΑ ΕΠΙΣΤΗΜΟΝΙΚΑ ΠΡΟΓΡΑΜΜΑΤΑ

1. **HPC – Europa 2** πρόγραμμα για τη μελέτη ιδιοτήτων υδατικών συστημάτων με χρήση κβαντικών μοριακών δυναμικών προσομοιώσεων.

   Φορέας: Ευρωπαϊκή Ένωση (2012).

   Επιστημονικός Υπεύθυνος: Dr Ioannis Skarmoutsos

   Συνεργάτης Φορέα Υποδοχής: Dr Marco Masia, University of Sassari, Department of Chemistry and Pharmacy.

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

   Πρόγραμμα εγκεκριμένο από το Science and Technology Facilities Council (STFC), United Kingdom (UK) (2016).

   Επιστημονικός Υπεύθυνος: Dr Sarantos Marinakis, Queen Mary University of London

   Συνεργάτης: **Dr Ioannis Skarmoutsos**

   Συνεργάτης: 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.**

   Πρόγραμμα εγκεκριμένο από τη Γενική Γραμματεία Έρευνας και Τεχνολογίας (GRNET) (2016).

   Επιστημονικός Υπεύθυνος: Dr Ioannis Skarmoutsos

   Επιστημονικός Υπεύθυνος: 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 ".

   Φορέας: Ευρωπαϊκή Ένωση (2019).

   Επιστημονικός Υπεύθυνος: Dr Ioannis Skarmoutsos

   Συνεργάτης Φορέα Υποδοχής: Professor Sofia Calero, Universidad Pablo de Olavide, Sevilla, Spain, Department of Physical, Chemical and Natural Systems.

ΕΓΚΕΚΡΙΜΕΝΕΣ ΕΥΡΩΠΑΪΚΕΣ ΥΠΟΤΡΟΦΙΕΣ

• 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.

ΕΠΙΣΤΗΜΟΝΙΚΗ ΕΠΙΜΟΡΦΩΣΗ

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.

ΥΠΟΛΟΓΙΣΤΙΚΕΣ ΔΕΞΙΟΤΗΤΕΣ

Επιστημονικός Προγραμματισμός	Fortran 77/90, experience in Unix systems, Linux, Mac OS, Windows. **Use of High Performance Computing Systems** (HPC Imperial College, Grace-UCL, Mare Nostrum BSC Barcelona, CINECA, Julich Germany, Titan-USA)
MD-Monte Carlo κώδικες προσομοίωσης	Εκτεταμένη γνώση των προγραμμάτων μοριακής προσομοίωσης DL_POLY, Moscito, Moldy, Moliq-Dynamo, CADDS (Monte Carlo), RASPA (Monte Carlo), CPMD, CP2k, Gaussian, GaussView, Materials Studio.
Ανάπτυξη Επιστημονικού Λογισμικού	**Ανάπτυξη επιστημονικού λογισμικού για την ανάλυση μοριακών τροχιών μοριακών δυναμικών και Monte Carlo προσομοιώσεων,** για των υπολογισμό στατικών θερμοδυναμικών, δομικών αλλά και δυναμικών ιδιοτήτων μοριακών συστημάτων και νανοπορωδών υλικών.

ΔΙΔΑΚΤΙΚΗ ΕΜΠΕΙΡΙΑ – ΛΟΙΠΕΣ ΕΠΙΣΤΗΜΟΝΙΚΕΣ ΔΡΑΣΤΗΡΙΟΤΗΤΕΣ

Διδασκαλία Προπτυχιακών Φοιτητών (Χημείας-Φαρμακευτικής),Εργαστήριο Φυσικοχημείας, ΕΚΠΑ. (2 ακαδημαϊκά έτη)

Προπτυχιακών Φοιτητών (Χημείας), Theoretical Chemistry Laboratory (Imperial College London, UK) (2 ακαδημαϊκά έτη)

Μεταπτυχιακών Φοιτητών (Φυσικής), Τμήμα Φυσικής, Universitat Politecnica de Catalunya (UPC), Spain (1 ακαδημαϊκό έτος)

Διδασκαλία Προπτυχιακών Φοιτητών Χημείας ΕΚΠΑ στη χρήση ηλεκτρονικών υπολογιστών, χρήση λειτουργικού συστήματος Windows, εκμάθηση του Office, πλοήγησης στο Internet καθώς και χρήσης εξειδικευμένων προγραμμάτων για τη Χημεία (Εφαρμογές της Πληροφορικής στη Χημεία) (1 ακαδημαϊκό έτος).

Κριτής σε 27 διεθνή επιστημονικά περιοδικά: *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, Frontiers in Physics-Condensed Matter Physics, Materials Today Communications, ACS Omega*
Κριτής της Γενικής Γραμματείας Έρευνας και Τεχνολογίας (GRNET) για επιστημονικά προγράμματα που σχετίζονται με επιστημονικούς υπολογισμούς σε υπερυπολογιστικές εγκαταστάσεις Υψηλής Απόδοσης (High Performance Computing Services)
Κριτής της Εθνικής Επιτροπής Έρευνας της Γαλλίας (ANR: Agence Nationale de la Reserche, https://anr.fr/en/) για την αξιολόγηση ερευνητικών προτάσεων προς χρηματοδότηση.
Μέλος της *European Molecular Liquids Group* (EMLG) .
Μέλος της συντακτικής επιτροπής (editorial board) του *Frontiers in Physics, Condensed Matter Physics* (Frontiers Media, Lausanne, Switzerland) από τις 07-11-2020.
Μέλος της συντακτικής επιτροπής (editorial board) του *Journal of Theoretical Chemistry* (Hindawi Publishing Corporation) κατά την περίοδο 28-11-2012 έως 23-07-2017.

ΓΛΩΣΣΟΜΑΘΕΙΑ

Ελληνικά (μητρική), Αγγλικά (άπταιστα, εργασιακή εμπειρία), Ισπανικά (πολύ καλά, εργασιακή εμπειρία), Γαλλικά (καλά, εργασιακή εμπειρία)

ΣΥΣΤΑΤΙΚΕΣ ΕΠΙΣΤΟΛΕΣ

Συστατικές επιστολές μπορούν να ζητηθούν από τους κάτωθι ακαδημαϊκούς ερευνητές:

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. Elvira Guardia
Departament de Física i Enginyeria Nuclear, Universitat Politècnica de Catalunya, Edifici B4-B5, Campus Nord, Jordi Girona 1-3, 08034 Barcelona, Spain
Email: elvira.guardia@upc.edu
Web page : http://simcon.upc.edu/usr/elvira.guardia

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

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
Former President of the Royal Society of Chemistry, former Dean of the Faculty of Natural Sciences, Imperial College of Science, Technology and Medicine, Exhibition Rd, South Kensington, London, SW7 2AZ, United Kingdom
Email : t.welton@imperial.ac.uk

Prof. Giancarlo Franzese
Departament de Física de la Matèria Condensada & Institut de Nanociència i Nanotecnologia (IN2UB), Universitat de Barcelona
Email: gfranzese@ub.edu
Web page : https://spcmub.wordpress.com/

ΥΠΟΜΝΗΜΑ

Δημοσιεύσεις σε διεθνή επιστημονικά περιοδικά με κριτές

47) **Local intermolecular structure, hydrogen bonding and related dynamics in the liquid cis/trans N-methylformamide mixture: A density functional theory based Born-Oppenheimer molecular dynamics study.**

Ioannis Skarmoutsos, Ricardo L. Mancera, Stefano Mossa and Jannis Samios, *J. Mol. Liq.* **365**, 120085 (2022)

46) **Fingerprints of the Crossing of the Frenkel and Melting Line on the Properties of High-Pressure Supercritical Water.**

Ioannis Skarmoutsos, Jannis Samios and Elvira Guardia *J. Phys. Chem. Lett.* **13**, 7636 (2022)

45) **Using Car-Parrinello simulations and microscopic order descriptors to reveal two locally favored structures with distinct molecular dipole moments and dynamics in ambient liquid water.**

Ioannis Skarmoutsos, Giancarlo Franzese and Elvira Guardia, *J. Mol. Liq.* **364**, 119936 (2022)

44) **A Computational Study on Phenyldiboronic Acid-Pillared Graphene Oxide Frameworks for Gas Storage and Separation.**

Ioannis Skarmoutsos, Emmanuel N. Koukaras, and Emmanuel Klontzas, *ACS Appl. Nano Mater. (accepted : June* 2022)

43) **CF_4 Capture and Separation of CF_4–SF_6 and CF_4–N_2 Fluid Mixtures Using Selected Carbon Nanoporous Materials and Metal–Organic Frameworks: A Computational Study.**

Ioannis Skarmoutsos, Emmanuel N. Koukaras, and Emmanuel Klontzas, *ACS Omega* **7**, 6691 (2022)

42) **On the Different Faces of the Supercritical Phase of Water at a Near-Critical Temperature: Pressure-Induced Structural Transitions Ranging from a Gaslike Fluid to a Plastic Crystal Polymorph**

Ioannis Skarmoutsos, Andres Henao, Elvira Guardia and Jannis Samios, *J. Phys. Chem. B* **125**, 10260 (2021)

41) **The Polar Cosolvent Effect on Caffeine Solvation in Supercritical CO_2–Ethanol Mixtures: A Molecular Modeling Approach.**

Ioannis Skarmoutsos, Ioannis D. Petsalakis and Jannis Samios, Ind. Eng. Chem. Res. **60**, 11834 (2021)

40) **The Impact of Ionic Liquid Loading in Three-Dimensional Carbon Nanotube Networks on the Separation of CO_2/CH_4 Fluid Mixtures: Insights from Molecular Simulations.**

Ioannis Skarmoutsos, Emmanuel N. Koukaras, and Emmanuel Klontzas, *J. Phys. Chem. C* **125**, 13508 (2021)

39) **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)

38) **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)

37) **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)

36) **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)

35) **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)

34) **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)

33) **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)

32) **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)

31) **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)

30) **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)

29) **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)

28) **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)

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

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

26) **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)

25) **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)

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

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ΠΑΡΟΥΣΙΑΣΕΙΣ

ΔΙΑΛΕΞΕΙΣ ΕΠΕΙΤΑ ΑΠΟ ΠΡΟΣΚΛΗΣΗ

17) **Molecular Simulations: A computational physical chemistry toolbox to predict, understand and rationally tailor the properties of molecular/ionic solvents and materials for sustainable chemical applications**

Ioannis Skarmoutsos, Invited Lecture at the Chemistry Department, University of Athens, Greece (2021)

16) **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)

15) **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).

14) **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).

13) **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).

12) **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)

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

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ΟΜΙΛΙΕΣ ΣΕ ΣΥΝΕΔΡΙΑ

17) **The unique structural features of water, ranging from ambient liquid up to supercritical, extreme-pressure conditions: Insights from classical and ab initio molecular dynamics simulations.**

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16) **Understanding the interactions of water with nanoporous materials to develop environmental** 1) **Gas storage and separation using three-dimensional pillared graphene oxide frameworks with phenyldiboronic acid linkers: A computational approach.**

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ΠΑΡΟΥΣΙΑΣΕΙΣ ΠΟΣΤΕΡ ΣΕ ΣΥΝΕΔΡΙΑ

19) **Fingerprints of the crossing of the Frenkel and Melting lines in high-pressure supercritical water.**

Elvira Guardia, Ioannis Skarmoutsos, Jannis Samios

European/Japanese Molecular Liquids Group-EMLG/JMLG Conference entitled: *"Molecular liquids at interfaces."* in Barcelona- Spain (2022)

18) **Confined Ionic Liquids (IL) in carbon-based materials for CO_2/CH_4 separation: insights from computer simulations.**

Ioannis Skarmoutsos, Emmanuel Klontzas, Emmanuel N. Koukaras

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17) **F-gas adsorption in pillared graphene materials. Insights from molecular simulations.**

Ioannis Skarmoutsos, Emmanuel Klontzas, Emmanuel N. Koukaras

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16) **Role of the Loading of Ionic Liquid $[EMIM]^+[BF_4]^-$ on the Separation of CO2/CH4 in 3D Carbon Nanotube Networks**

I. Skarmoutsos, R. Lingas, E.N. Koukaras, E. Klontzas

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15) **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

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

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

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

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

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

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7) **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

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

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5) **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.**

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

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