Δρ. ΙΩΑΝΝΗΣ ΣΚΑΡΜΟΥΤΣΟΣ

Γεννηθείς στα Βασιλικά Φθιώτιδας, Ελλάδα

Ημερομηνία Γέννησης: 28 Μαρτίου 1977

Υπηκοότητα: Ελληνική

Email: iskarmoutsos@uoi.gr

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 23-02-2025
- **53 Δημοσιεύσεις** σε Διεθνή περιοδικά με κριτές (βλ. Υπόμνημα)
- **h-index: 22** (Πηγή: Google Scholar)
- **i10-index: 34** (Πηγή: Google Scholar)
- **1** δημοσίευση σε κεφάλαιο επιστημονικού βιβλίου (βλ. Υπόμνημα)
- **4** Δημοσιεύσεις σε βιβλία πρακτικών συνεδρίων (βλ. Υπόμνημα)
- **2** Αναδημοσιευμένες εργασίες (βλ. Υπόμνημα)
- **19** Διαλέξεις έπειτα από πρόσκληση (βλ. Υπόμνημα)
- **19** Παρουσιάσεις Πόστερ σε συνέδρια (βλ. Υπόμνημα)
- **22** Ομιλίες σε συνέδρια (βλ. Υπόμνημα)
- **4** Εγκεκριμένα Ερευνητικά Προγράμματα
- **1** Εγκεκριμένη Διεθνής Ερευνητική Υποτροφία

ΕΓΚΕΚΡΙΜΕΝΑ ΕΠΙΣΤΗΜΟΝΙΚΑ ΠΡΟΓΡΑΜΜΑΤΑ (ΠΡΙΝ ΤΗΝ ΕΚΛΟΓΗ ΜΟΥ ΩΣ ΕΠΙΚΟΥΡΟΥ ΚΑΘΗΓΗΤΗ)

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.

ΕΓΚΕΚΡΙΜΕΝΑ ΕΠΙΣΤΗΜΟΝΙΚΑ ΠΡΟΓΡΑΜΜΑΤΑ (ΜΕΤΑ ΤΗΝ ΕΚΛΟΓΗ ΜΟΥ ΩΣ ΕΠΙΚΟΥΡΟΥ ΚΑΘΗΓΗΤΗ)

Συμμετοχή σε Ευρωπαϊκά Συνεργατικά Ερευνητικά Προγράμματα ως επιστημονικός εταίρος

1. **MUSICODE project** (https://musicode.eu/), " *An experimentally-validated multi-scale materials, process and device modeling & design platform enabling non-expert access to open innovation in the organic and large area electronics industry*"

   European collaborative research and innovation project led by a multi-disciplinary consortium coordinated by University Ioannina. I started participating in the project on 2022.

Συμμετοχή σε Ελληνικά Συνεργατικά Ερευνητικά Προγράμματα ως επιστημονικός εταίρος

2. Εμβληματικές δράσεις σε διαθεματικές επιστημονικές περιοχές με ειδικό ενδιαφέρον για την σύνδεση με τον παραγωγικό ιστό: "*7.1 Ανάπτυξη αποδοτικών ΦΒ υλικών και διατάξεων τρίτης γενιάς για την ενίσχυση της ανταγωνιστικότητας του παραγωγικού τομέα στην πράσινη ενέργεια*"

Πρόγραμμα Εγκεκριμένο το 2023

https://gsri.gov.gr/istoselides-enischyomenon-ergon/

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	Fortran 77/90, Python, experience in Unix systems, Linux, Mac OS, Windows.
Προγραμματισμός	**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

Πριν την εκλογή μου ως επίκουρου καθηγητή

1) 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)**.
2) Διδασκαλία Προπτυχιακών Φοιτητών (Χημείας-Φαρμακευτικής),Εργαστήριο Φυσικοχημείας, ΕΚΠΑ. **(2 ακαδημαϊκά έτη)**
3) Προπτυχιακών Φοιτητών (Χημείας), Theoretical Chemistry Laboratory (Imperial College London, UK) **(2 ακαδημαϊκά έτη)**
4) Σεμινάρια στατιστικής μηχανικής και τεχνικών μοριακής προσομοίωσης σε μεταπτυχιακούς φοιτητές, Τμήμα Φυσικής, Technical University of Catalonia (**1 ακαδημαϊκό έτος**)

Μετά την εκλογή μου ως επίκουρου καθηγητή στο Πανεπιστήμιο Ιωαννίνων

1) Διδασκαλία προπτυχιακού μαθήματος "Φυσικοχημεία Ι" (Κλασική Θερμοδυναμική)Τμήμα Χημείας, Πανεπιστήμιο Ιωαννίνων (**Ακαδημαϊκά Έτη 2022-2023, 2024-2025**)
2) Δημιουργία και Διδασκαλία της νέας ύλης του προπτυχιακού μαθήματος και εργαστηρίου "Η/Υ-Πληροφορικής" με έμφαση στον "Προγραμματισμό σε γλώσσα Python" , Τμήμα Χημείας, Πανεπιστήμιο Ιωαννίνων (**Ακαδημαϊκά Έτη 2022-2023, 2023-2024, 2024-2025**)
3) Διδασκαλία πειραματικών εργαστηριακών ασκήσεων στο πλαίσιο του προπτυχιακού "Εργαστηρίου Φυσικοχημείας Ι", Τμήμα Χημείας, Πανεπιστήμιο Ιωαννίνων, (**Ακαδημαϊκά Έτη 2022-2023, 2023-2024, 2024-2025**)
4) Εισαγωγή και διεξαγωγή νέων ασκήσεων Υπολογιστικής Φυσικοχημείας (Άσκηση 1: Υπολογισμός Ενθαλπίας Εξάτμισης και Δεσμών Υδρογόνου του Υγρού νερού μέσω μοριακής δυναμικής προσομοίωσης, Άσκηση 2: Υπολογισμός Μερικών Γραμμομοριακών Όγκων και Δεσμών Υδρογόνου σε υγρά μίγματα νερού-προπανόλης-1) στο πλαίσιο του προπτυχιακού "Εργαστηρίου Φυσικοχημείας Ι", Τμήμα Χημείας, Πανεπιστήμιο Ιωαννίνων
(**Ακαδημαϊκά Έτη 2023-2024, 2024-2025**)
5) Συμμετοχή στη διδασκαλία του προπτυχιακού μαθήματος επιλογής του 4ου έτους: "Έννοιες Χημείας" , Τμήμα Χημείας, Πανεπιστήμιο Ιωαννίνων (**Ακαδημαϊκό Έτος 2023-2024**)

Ακαδημαϊκός Επιβλέπων Μεταπτυχιακών και Προπτυχιακών Φοιτητών/τριών:

Επιβλέπων του μεταπτυχιακού φοιτητής κ. Ηλία Καρβούνη (Τμήμα Χημείας, Πανεπιστήμιο Ιωαννίνων, Υποστήριξη Μεταπτυχιακής Διατριβής: Σεπτέμβριος 2024)

Επιβλέπων 7 προπτυχιακών φοιτητών/τριών για εκπόνηση πτυχιακής εργασίας (4 πτυχιακές εργασίες έχουν ολοκληρωθεί, 3 σε εξέλιξη).

Μέλος της τριμελούς συμβουλευτικής επιτροπής 2 Υποψηφίων Διδακτόρων
Μέλος της επταμελούς εξεταστικής επιτροπής 3 Υποψηφίων Διδακτόρων.

Μέλος της τριμελούς συμβουλευτικής επιτροπής 1 μεταπτυχιακής φοιτήτριας.
Συνεπιβλέπων ενός μεταδιδακτορικού ερευνητή (στο πλαίσιο του ευρωπαϊκού ερευνητικού προγράμματος Musicode, https://musicode.eu/ , σε συνεργασία με τον καθηγητή κ. Ελευθέριο Λοιδωρίκη, Τμήμα Μηχανικών Επιστήμης Υλικών, Πανεπιστήμιο Ιωαννίνων)

ΛΟΙΠΕΣ ΕΠΙΣΤΗΜΟΝΙΚΕΣ ΔΡΑΣΤΗΡΙΟΤΗΤΕΣ

Κριτής σε 32 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 CO2 Utilization, Frontiers in Physics-Condensed Matter Physics, Materials Today Communications, ACS Omega, Langmuir, Computational and Theoretical Chemistry, Separation and Purification Technology, Physical Review Research, Scientific Reports*

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
Former Assistant Professor of Theoretical Chemistry, Dipartimento di Chimica, Università degli studi di Sassari, Via Vienna 2, 07100, Sassari, Italy
Currently: Head of Entrepreneurship, University of Vienna, Austria
Email: marco.masia@univie.ac.at

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
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ΥΠΟΜΝΗΜΑ

Δημοσιεύσεις σε διεθνή επιστημονικά περιοδικά με κριτές

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49) **Solvation structure and dynamics of favipiravir in supercritical CO2. A molecular dynamics investigation.**

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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**

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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.**

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ΠΑΡΟΥΣΙΑΣΕΙΣ

ΔΙΑΛΕΞΕΙΣ ΕΠΕΙΤΑ ΑΠΟ ΠΡΟΣΚΛΗΣΗ

19) **Molecular Simulations: A computational toolbox to predict, understand and rationally tailor the physicochemical properties of liquid and supercritical solvents and materials for sustainable chemical applications.**

Ioannis Skarmoutsos, Invited Lecture at the Institute of Physics, Polish Academy of Sciences, Warsaw, Poland (2024)

18) **Using classical and ab initio molecular dynamics, statistical mechanical theories and structural order parameters to study the phase-behavior of molecular systems: The unique case of water at ambient-pressure liquid up to extreme-pressure supercritical thermodynamic conditions.**

Ioannis Skarmoutsos, Invited Lecture at the Department of Materials Science and Engineering, University of Ioannina, Workshop on Computational Materials Science organized by Department of Materials Science and Engineering, University of Ioannina and the Hellenic Society for the Science and Technology of Condensed Matter (HSSTCM).

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)

11) **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)

10) **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)

9) **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)

8) **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)

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

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

6) **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)

5) **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)

4) **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)

3) **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).

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

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1) **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)

ΟΜΙΛΙΕΣ ΣΕ ΣΥΝΕΔΡΙΑ

22) **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.**

23rd Panhellenic Chemistry Conference, Athens-Greece (2024)

21) **Pillared graphene oxide frameworks for the adsorption and separation of dimethylsulfoxide-water mixtures.**

European/Japanese Molecular Liquids Group-EMLG/JMLG Conference entitled: *"Structure and Dynamics of Hydrogen-Bonded Systems."* in Trieste- Italy (2024)

20) **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.**

2nd International Conference on Physical Chemistry and Spectroscopy (ICPCS), Patras, Greece (2023)

19) **Solvation structure and dynamics of pharmaceutical compounds in liquid and supercritical solvents: The cases of caffeine and favipiravir.**

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European Conference of Computational & Theoretical Chemistry, EuChems CompChem in Thessaloniki, Greece (2023)

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.**

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

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.**

Graphene 2021 Conference, Grenoble, France (2021)

15) **SF_6 Capture and Separation of SF_6-N_2 Fluid Mixtures Using Porous Carbon Nanotube Networks and Pillared Graphene Materials**

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14) **The different faces of the supercritical phase of water at a near-critical temperature.**

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

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

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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

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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

35^{th} Panhellenic Conference on Solid State Physics and Materials Science, Athens, Greece (2021)

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

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.

14) **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

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

Ioannis Skarmoutsos, Stefano Mossa and Jannis Samios

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

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

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

Ioannis Skarmoutsos, Elvira Guardia and Jannis Samios

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10) **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

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

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