
Professor Dr Jannis SAMIOS
●**Director of Physical Chemistry Laboratory**
●**Head of Section I**
**Sector:** Physical & Theoretical Chemistry
Department of Chemistry
National University of Athens (UoA)- Greece
Phone: **+30 210 7274534, 7274751 (office)**
Fax: **+30 210 7274752**
Email: **isamios @chem.uoa.gr** Web page http://users.uoa.gr/~jsamios/


# CURRICULUM VITAE

## PERSONAL DATA

**FULL NAME:** **Jannis Nicolaos SAMIOS**

**NATIONALITY**: GREEK

**DATE OF BIRTH**: Limni Evias, 1949,
Married, two children

**ADDRESSES**:

**Office Address**: **"***National & Kapodistrian University of Athens, Department of Chemistry, Laboratory of Physical &Theoretical Chemistry, Panepistimiopolis 157 71, Athens, Greece".*

**Home Address:** 11, Orfanidou st, Marousi, GR-15126, Athens Greece:
Tel.: +30 210 8065030

**Military Service**, June1973 - December 1975 (Greek Air Forces)

## Academic Qualifications:

- **PhD**, *Department of Chemistry, Laboratory of Physical Chemistry I, University Bielefeld-Germany (1976-1981)*

*"Physical Chemistry& Chemical Physics Studies in Liquid State Molecular Systems via Statistical Mechanical Theory, Spectroscopy & Computer Simulation Computational Techniques"*

- **B.Sc**., *Faculty of Physical & Mathematical Science, Departent of Mathematics, National & Kapodistrian Uuniversity of Athens-Greece (1973)*

## Appointments: Employment & Experience

- September 2006-today: **Professor.** Chemistry Department, University of Athens-Greece

- September 2006-1993: **Associate Professor**, Chemistry Department, Univ. of Athens

- 1993-1988: **Assistant Professor**, Chemistry Department, University of Athens

- 12/1989-1/1986: **Postdoctoral Researcher** "Institute Physical Chemistry II, University Bielefeld & *Centrum for Interdisciplinary Research* (ZIF) Nordr. Westfalen, awarded by "*Deutsche-Forschungsgemeinschaft (DFG)"*

- 12/1985-1/1982: **Postdoctoral Research & Teaching & Ass**.(Pos. BaT II) "Department of Chemistry, Institute. PC II, University Bielefeld, Germany

- 12/1981-3/1976: **Teaching & Research Associate** " Department of Chemistry, Insitute PC I & II, University Bielefeld, Germany (by Profs. Dr **Dorfmüller**, **Jost** and **Knoche**)

- Autumn 1978: **Visiting Research Fellow**, Chemistry Department, Royal Holloway College, University of London U. K. , Institute of Physical Chemistry & Molecular Physics (by Prof. **K. Singer**)

## Teaching Activities: *Classes taught*

• For Undergraduate & Post-graduate students:

•Computer programming and applications in FORTRAN & C, UNIX

•Mathematics & Statistics, Special Mathematical Techniques in Computational Physical Chemistry.

•Kinetic Theory & Transport Properties of particles.

•Classical & Statistical Thermodynamics.

•Statistical Molecular Mechanics-Linear response theory - Time correlation Functions & Relaxation Phenomena-Pair Distribution Functions & Intermolecular Structure

•Intermolecular forces based upon *Effective Potential Models* between Molecules in Condensed Matter Molecular Systems (liquids, Supercritical fluids etc. .)

•Computer Simulation Techniques Monte Carlo & Molecular Dynamics, Molecular Mechanics,
etc…..

**Supervisor**: of 9 PhD Dissertations, 15 M.Sc Theses, 24 Diploma Theses

## Research Interests/Activities:

• ***Physical Chemistry Science*** *of Dense Molecular Systems-*
*Molecular Liquids & Supercritical Fluids*
•***Statistical Mechanics & Thermodynamics***-Theoretical Methods & Applications via (Analytical Theory, **DFT**, **PY, HC, RISM, MSA, MF, MMK**, etc.) –investigation of the structural & dynamical aspects of the condensed matter molecular systems.
•***Computer Modeling*** of Molecular Systems using Computational Simulation Techniques (MD, MC, MM, etc..).

**Research Topics of Interest:**

• Physico - Chemical & Chemical Physics Studies of:

•Simple & complex molecular liquid systems (pure & solutions)

•Supercritical fluids-(pure and mixtures) (alternative non toxic solvents-Applications in Green Chemistry) etc..

• Studies of the intermolecular forces in molecular systems and construction of effective potential models among the molecules.

• Theoretical-computational studies on the properties of ionic liquids and surfactants.

• Theoretical-computational studies of interaction induced phenomena in molecular liquid systems.

• *Aspects on various gases* ($H_2$ , $CO_2$ etc.) uptake on specific molecular substrates (Carbon Nanotubes CNTs, Silicon Carbon NTs, MOFs etc..)

• Participation in 40 national & international conférences (Invited talks 35, Oral presentations 20, Session chair 18, Posters 30)

## Scientific

### Publications/Citations:

•(70) Publications in international Journals • (30) conference papers • (8) Invited papers in International Journals.

•**Main Organizer & Editor**-Special Vol. *NATO ASI Science Series* II Mathematics, Physics & Chemistry Kluwer Academic. Publication (2004)"*Novel Approaches to the Structure and Dynamics of Liquids*"

•**Guest Editor**-Special Issue "*Journal of Molecular Liquids"* (2004) [Annual Conference (European Molecular Liquid Group (EMLG)& Japanese Molecular Liquid Group (JMLG)]

•**Guest Editor**-Special Issue in "*J.Pure & Applied Chemistry (IUPAC)* (2004) *(EMLG* – JMLG) *Rhodes meeting)*

•**Main Organizer**» of the Annual Meeting of the *EMLG/JMLG* international Scientific Societies, **which be held** in **Crete – Chania, Greece** (11 -16 September 2016).
**Title** "*Progresses on the Experimental & Theoretical-Computational Techniques for the Study of Liquids and Supercritical Fluids. From Simple to Complex Systems"*

•More than 1000 citations. (H-index19)

## Distinctions-Awards

• 3/1976-12/1981: Ph.D Fellowship, DFG, ZIF – Germany.

•"Certificate of Appreciation" from EMLG/JMLG Scientific Societies as main organizer for the conference & summer school-Rhodes 2002.

•Awarded (sponsored) by IUPAC-as main organizer of the "Annual Meeting of EMLG/JMLG international Scientific Sociaties.

•Awarded (sponsored) by NATO-as main organizer of the NATO-ASI summer school

2002. • Awarded from the "*International Scientific-Exchange Program, Collaborative Research Grant- NATO, (Univ. Athens Greece, Techn. Univ. Aachen & Penn State University USA)".*

• Awarded (sponsored.) by the *Chemical Industry of Germany (Fonds der Deutsche. Chemischen Industrie)* • Awarded (sponsored) by the German Automobile Industry (Volkswagenwerk Stiftung), etc….
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## Other Activities:

• **Member of** the
• International Advisory Committee "*European Molecular Liquid Group (*EMLG)

•Editorial Board of the *Journal of Molecular Liquids*

•*Deutshe Bunsen Gesellschaft Physikalische Chemie*

•*Greek union for hydrogen technologies (ELETY)*

• **Reviewer of**:

• Proposals submitted for evaluation in.-GSRT of Greece & other national & international found/s & organ/s

• Scientific papers submitted for evaluation. in *JCP, JPC A, JPC B, JPC C, JPC L, Chem. Phys., Che. Phys.L., JML, EPJ, J. Exp. Nanosien., Intr. J. Hydr. Ener. etc.*

• Proposals submitted for evaluation in PRACE, Scientific Review (Partnership for Advanced. Super Computer Facilities in Europe)
• Management of 10 research projects and participation in 4 infrastructure projects. Scientist in Charge in 12 research proposals

## Publications

### • Dissertation

*(Dissertation zur Erladung des Doktorgrades der NATURWISSSENSCHAFTEN (DR.RER.NAT) der Facultät für Chemie - Physicalishe Chemie an der Universität. BIELEFELD -GERMANY)*
**Jannis Samios** Department of Chemistry, University of Bielefeld Germany (**1981**)

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• *"Collision effects in liquid $CCl_4$ . A molecular dynamics study".*

**J. Samios** and **Th. Dorfmüller**

**Journal of CHEMICAL PHYSICS** 76, 5463 (1982)

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• *"Molecular Dynamics of liquid Argon: Collision times and Durations"*

**J. Samios, D. Samios, W. Mersch, Th. Dorfmüller**

**Ber. Bunsenges. PHYSICAL CHEMISTRY** (Germany)86, 52 (**1982**)

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•*"Collision-Induced absorption in non polar molecular liquids".*

**H. Arning, J. Samios, K. Tibulski, Th. Dorfmüller**

**Chemical Physics** 67, 177 (**1982**)

• *"Application of the Mode-Matching Model to V-T (Vibration - Translation) in liquid $CCl_4$"*

**D. Samios, J. Samios, Th. Dorfmüller**

**Molecular Physics** 49, 543 (**1983**)

- *"A Molecular Dynamics Simulation of interaction induced dipole correlation functions in liquid $CS_2$".*

**Th. Dorfmüller, J. Samios**

**Molecular Physics** 53, 1167 (**1984**)

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- *"Steric Hindrance of Diffusion controlled reactions".*

**M. Lopez-Quintella, J. Samios, W. Knoche**

**Journal of Molecular Liquids** 29, 243 (1984)

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- *"The FAR-INFRARED absorption spectrum of liquid $N_2$. A molecular dynamics simulation study".*

**J. Samios, U. Mittag, Th. Dorfmüller**

**Molecular Physics** 56, 541 (**1985**)

---

- *"Interaction - induced Far-Infrared spectra of liquid $CS_2/CCl_4$ mixtures".*

**M. Potthast, J. Samios, Th. Dorfmüller**

**Chemical Physics** 102, 147 (**1986**)

---

- *"A Molecular Dynamics Simulation of interaction-Induced FAR-INFRARED absorption spectra of liquid $CS_2$ ".*

**J. Samios, U. Mittag, Th. Dorfmüller**

**Molecular Physics** 59, 65 (**1986**)

- *"Octopole and Hexadecapole induction mechanisms in interaction - induced spectra: A Molecular Dynamics Simulation."* .

**Th. Dorfmüller, J. Samios, U. Mittag**

**Chemical Physics** 107, 397 (1986)

---

- *"Brownian motion and Fractal geometry in liquid state. I. Translations of linear Molecules".*

**J. Samios, P. Pfeifer, M. Obert, U. Mittag, Th. Dorfmüller**

**Chemical Physics Letters** 123, 545 (**1986**)

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- *"Translational correlation functions of interaction induced dipoles in dense media".*

**Z. Gburski, J. Samios, Th. Dorfmüller**

**Journal of CHEMICAL PHYSICS** 86, 383 (**1987**)

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- *"Influence of Fractal Dimension on diffusion controlled reactions".*

**M. Lopez-Quintella, J. Moure, M. Nunez, J. Samios**

**Chemical Physics Letters** 138, 476(**1987**)

---

- *"Translational component of the interaction-induced dipole correlation functions in dense fluids".*

**Z.Gburski, J. Samios, Th. Dorfmüller**

**Journal of CHEMICAL PHYSICS** 87, 7348 (**1987**)

---

- *"Molecular Dynamics Simulation of the liquid mixture $CCl_4/CS_2$. I.Thermodynamics and Structural properties".*

**U. Mittag, J. Samios, Th. Dorfmüller**

**Molecular Physics** 66, 51 **(1989**)

• *"A Comparative MOLECULAR DYNAMICS and NEUTRON SCATTERING study of the structural …..of the binary mixture $CCl_4/CS_2$".*

**U. Mittag, J. Samios, Th. Dorfmüller, St. Gunster, U. Zeidler Chieux**

**Molecular Physics** 67, 1141 (**1989**)

---

• "*Concentration effects on collision induced Depolarized Rayleigh line shapes in $CCl_4/CS_2$ liquid mixture".*

**F. Strehle, Th. Dorfmüller, J. Samios**

**Molecular Physics** 72, 933, (**1990**)

---

• "*Molecular Dynamics Simulation of Depolarized Rayleigh and Far - infrared spectra in binary liquid mixtures".*

**H. Stassen, U. Mittag, J. Samios**

**NATO Advanced Study Inst**., Series C: Mathem. and Phys. Sciences – Luso Portugal, Sep.1991.Thema:"Molecular Liquids, New Perspectives in Physics and Chemistry". NATO ASI Series C Vol. 379, Kluwer, Academic Publishers, Dordrecht. Edited by **Jose J. C. Texeira-Dias:**Vol. 379, p. 549-568 (Publ. 1992)

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•*"Concentration dependent FAR-infrared absorption spectra of the mixtures FURAN/$CS_2$, FURAN/$CCl_4$, FURAN/$C_6H_6$".*

**M. Haritopoulou, J. Samios, E. Zoidis, Th. Dorfmüller**

**Ber. Bunsenges. PHYSICAL CHEMISTRY** (Germany) 95, 1637(**1991**)

---

• *"Molecular dynamics simulation of liquids with $T_d$, $O_h$ molecular symmetry. A two model potentials approach".*

**H. Stassen, J. Samios, Th. Dorfmüller**

**Molecular Simulation** 8, 215 (**1992**)

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- *"Test of effective pair potential models by Molecular Dynamics Simulation on liquid OCS".*

**J. Samios, H. Stassen, Th. Dorfmüller**

**Chemical Physics** 160, 33 (**1992**)

---

- *"Molecular Dynamics Investigation of the Electrostatic interactions in liquid OCS"*

**H. Stassen, Th. Dorfmüller, J. Samios**

**Molecular Physics** 77, 339 (**1992**)

---

- *"Far - infrared interaction induced absorption spectra of $C_6H_6/CS_2$ liquid mixtures".*

**E. Zoidis, J. Samios, Th. Dorfmüller**

**Chemical Physics** 168, 349 (**1992**)

---

- *"Far - infrared absorption spectra of Thiophene in liquid solutions with $CS_2$".*

**M. Haritopoulou, J. Samios, D. Dellis, E. Zoidis**

**Chemical Physics** 169, 103 (**1993**)

---

- *"Time correlation functions of liquid OCS. A Molecular dynamics study".*

**J. Samios, H. Stassen**

**Chemical Physics** 170, 193 (**1993**)

---

- *"Density dependent structural properties of diluted mixtures OCS/Ar".*

**J. Samios, D. Dellis, H. Stassen**

**Chemical Physics** 178, 83 (**1993**)

---

- *"Molecular Dynamic Simulation of the liquid mixture $CCl_4/CS_2$ :*

*II. Concentration dependence of the translational and rotational motion".*

**U. Mittag, J. Samios , Th. Dorfmüller**

**Molecular Physics** 81, 1143 (**1994**)

---

- *"Estimation of the cancellation effects in interaction induced FIR spectra of liquid mixtures via MD simulation. Application....." .*

**J. Samios, U. Mittag**

**Journal of PHYSICAL CHEMISTRY** 98, 2033 (**1994**)

---

- *"Dynamical properties of Carbonyl Sulphide diluted in Argon at different densities. A Molecular Dynamics Investigation"*

**J. Samios, D. Dellis**

**Chemical Physics** 192, 281 (**1995**)

---

- *"Density dependence of the structural properties and translational diffusion of Carbonyl Sulphide diluted in mono atomic solvents. A Molecular Dynamics investigation"*

**D. Dellis, J. Samios**

**Journal of Molecular liquids** 185, 70 (**1996**)

---

- *"Structural and Dynamical Properties of HCl Dissolved in $CCl_4$. A Molecular Dynamics Study"*

**G. Chatzis, J. Samios, M. Chalaris**

**Chemical Physics** 228,241 (**1998**)

---

- *"A Molecular Dynamics Simulation Study of LiCl diluted in DMF(-d7)"*

**M. Chalaris, J. Samios**

**Journal of Molecular Liquids** 78, 201 (**1998**)

---

• "Solvation and catalyst-substrate of a Tungsten tris (dithiolene) complex dissolved in water-acetone. A Molecular Dynamics Model Calculation"

**J. Samios, D. Katakis, D. Dellis, E. Lyris, C. Mitsopoulou**

**Journal Chem. Soc., Faraday Trans.,** 94, 3169 (**1998**)

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•*"Hydrogen Bonding in Supercritical Methanol.*
*A Molecular Dynamics Investigation"*

**M. Chalaris, J. Samios**

**Journal of PHYSICAL CHEMISTRY B** 103, 1161 (**1999**)

---

• **"***Systematic molecular dynamics studies of liquid N,N Dimethyl Formamide using optimized rigid force fields. Investigation of the thermodynamic, structural, transport and dynamic properties***"**

**M. Chalaris, J. Samios**

**Journal of CHEMICAL PHYSICS** 112, 8581 (**2000**)

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• *"The Isotopic and Temperature Dependent Properties of Hydrogen Chloride Diluted in Carbon Tetrachloride. A molecular Dynamics Approach."*

**G. Chatzis, J. Samios**

**Chemical Physics** (Elsevier) 257, 51 (**2000**)

---

• "*Computer simulation studies of the liquid mixtures water-dimethylsulfoxide using different effective potential models: Thermodynamic and transport properties''*

**M. Chalaris, J. Samios**

**Journal of Molecular Liquids** 98, 399 (**2001**)

- *"Estimation of the Interaction-Induced Effects on the Formation of the Far-infrared and Infrared Correlation Functions of HCl dissolved in $CCl_4$: A Molecular Dynamics Study"*

**G. Chatzis, J. Samios**

**Journal of PHYSICAL CHEMISTRY A** 105, 9522 (**2001**)

---

- "*Molecular Dynamics Simulations of the liquid mixtures N, N-dimethylformamide-water using available potential models"*

**M. Chalaris, A. Koufou, J. Samios**

**Journal of Molecular Liquids** 101, 69 **(2002**)

---

- *"Binary mixtures of supercritical carbon dioxide with methanol. A molecular dynamics simulation study"*

**G. Chatzis, J. Samios**

**Chemical Physics Letters** 374, 187 (**2003**)

---

- **"***Translational and rotational dynamics in supercritical methanol from molecular dynamics simulation"*

**M. Chalaris, J. Samios**

**Pure and Applied Chemistry** (Official Journal of IUPAC) 76, 203 (**2004**)

---

- **"***Molecular dynamics simulation of dilute aqueous DMSO solutions. A temperature-dependence study of the hydrophobic and hydrophilic behaviour around DMSO"*

**R. L Mancera, M. Chalaris, K. Refson, J. Samios**

**Phys.Chem.Chem.Physics (PCCP),** 6, 94 ( **2004**)

---

- *"Transport properties of diatomic ions in moderately dense gases in an electrostatic field"*

**A. D. Koutselos, J. Samios**

**Pure and Applied Chemistry** (Official Journal of IUPAC) 76, 223(**2004**)

- *"The concentration effect on the 'hydrophobic' and 'hydrophilic' behaviour around DMSO in dilute aqueous DMSO solutions. A computer simulation study"*

**R. L Mancera, M. Chalaris, J. Samios**

**Journal of Molecular Liquids** 110, 147 (**2004**)

---

- *"Molecular dynamics of cis/trans N-methylformamide liquid mixture using a new optimized all atom rigid force field"*

**I. Skarmoutsos, J. Samios**

**Chemical Physics Letters** 384, 108 (**2004**)

---

- "Special issue - Novel Approaches to the Structure and Dynamics of Liquids: Experiments, Theories and Simulations" - Meeting of the European and Japanese Molecular Liquid Groups (EMLG/JMLG) September 7-15, 2002, Rhodes, Greece - **Preface**

**P. A. Bopp, J. Samios, M. D. Zeidler**

***J. Molecular Liquids*** 110, 1 (**2004**)

---

- "European Molecular Liquids Group (EMLG) Annual Meeting on the Physical Chemistry of Liquids - Novel approaches to the structure, dynamics of liquids: Experiments, theories and simulation" - Held in Rhodes, Greece, 7-15 Sept. 2002 - **Preface**

**J. Samios, P. A. Bopp**
*Pure Applied. Chem.* **76**, V-VII (2004)

---

- **"***Recent Advances in the Understanding of Hydrophobic and Hydrophilic effects: A Theoretical and Computer Simulation Perspective"*

**R. L. Mancera, M. Chalaris, J. Samios**

**NATO Advanced Study Inst**., Series II: Mathematics, Physics and Chemistry. Rhodes Greece, Sep. 2002. Thema: " Novel approaches to the Structure and Dynamics of Liquids: Experiments, Theories and Simulations ". Edited by **Jannis Samios & Vladimir A. Durov**. Kluwer, Academic Publishers, Dordrecht, Vol. 133, p. 387-397. (Publ. 2004)

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- "*Hydrogen Bonding In Aqueous Mixtures Containing Aprotic Solvents:*

  **M. Chalaris, J. Samios**

**Lecture Series on Computer & Computational Sciences** Vol.1, 110 (2004)
*VSP International Science Publishers-Utrecht . Boston*
(Guest Editor. **G. Maroulis**) (Short Communication)

- **"***Monte Carlo simulation of Gas Adsorption in Single Walled Nanotubes"*

  **G. P. Lithoxoos, J. Samios**

**Lecture Series on Computer & Computational Sciences** Vol.1, 317 (2004)
*VSP International Science Publishers-Utrecht . Boston*
(Guest Editor. **G. Maroulis)**

- **"***Molecular Dynamics Simulation of Cis-Trans N-Methylformamide (NMF) Liquid mixture. Structure and dynamics"*

  **I. Skarmoutsos, J. Samios**

**Lecture Series on Computer & Computational Sciences** Vol.1, 479 (2004)
*VSP International Science Publishers-Utrecht . Boston*
(Guest Editor. **G. Maroulis)**

- *"Investigation of the vapor-liquid equilibrium and supercritical phase of pure Methane via computer simulations"*

  **I. Skarmoutsos, L. I. Kampanakis, J. Samios**

**Journal of Molecular Liquids** 117, 33 ( **2005**)

---

- *"The temperature and density dependence of fluid xenon self-diffusion coefficients: a comparison between experimental, theoretical and molecular dynamics results"*

  **S. Marinakis, J. Samios**
**The journal of Supercritical Fluids** 34, 81 (**2005**)

---

- **"***Pressure and Temperature Dependence of the Hydrogen Bonding in Supercritical Ethanol. A Computer Simulation Study"*
  **D. Dellis, M. Chalaris, J. Samios**

**Journal of PHYSICAL CHEMISTRY B** *10,* 18575 (**2005**)

- "Local intermolecular structure, density inhomogeneities and dynamics in binary supercritical solutions. A Molecular Dynamics Simulation study of methane in carbon dioxide.

**I. Skarmoutsos, J. Samios**
**Journal of Molecular Liquids** 125, 181, **(2006)**

---

- *"* SiC nanotubes: A novel material or hydrogen storage*"*,

**Mpourmpakis G, Froudakis G, Lithoxoos G, Samios J.**

***Nano Letters*** *6*, 1581, (**2006)**

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- *"*Local density inhomogeneities and dynamics in….A molecular dynamics simulation approach*"*,

**Skarmoutsos I, Samios J.**
***J. Phys. Chemistry B***. *11*, 21931 (**2005)**

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- *"* Local density augmentation and dynamics….supercritical fluids. A molecular…",

**Skarmoutsos I, Samios J.**
***J. Chemical Physics***. *126*, 044503.**(2007)**

---

- "Effect of curvature and chirality for hydrogen storage in carbon nanotubes. A combined**…",**

**Mpourmpakis G, Froudakis G, Lithoxoos G, Samios J**
***J. Chemical Physics***. *126*, 144704. **(2007)**

---

- "The investigation of the local composition enhancement …in super critical CO2-cosolvent mixtures…",

**Skarmoutsos I, Dellis D**, **Samios J**

***J. Chemical Physics*** *126*, 224503 (**2007**)

---

- "New effective method for quantitative analysis of diffusion…..of small molecules….",

**Raptis T. E, Raptis V, Samios J**

**J. Physical Chemistry B,** 11, 13683 **(2007)**

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- "Investigation of Silicon Model Nanotubes as potential Nanomaterials for Efficient…….H2 storage…",

**Lithoxoos G, Samios J, Carrisan Y**

**J. Physical Chemistry C,** 11, 16725 **(2008)**

---

- "The effect of intermolecular interactions on local density inhomogeneities ……Simulation study"

**Skarmoutsos I, Dellis. D, Samios J.**

***J. Phys. Chemistry B*** *113*, 2783 (**2009**)

---

- "Conformational and Solvation studies via Computer Simulation of the Novel Large Scale Diastereoselectively Synthesized phosphinic MMP Inhibitor RXP03 Diluted in Selected Solvents",

**M. Matziari, Dellis, V. Dive, A. Yiotakis and J. Samios,**
***J. Physical Chemistry B*** *14*, 421 (**2010**)

---

- "Hydrogen bond, electron donor-acceptor dimer, H-bond residence dynamics in supercritical CO2-ethanol mixtures and the effect of hydrogen bonding on single reorientational and translational dynamics. A molecular dynamics imulation study."

**Skarmoutsos I., Guardia E**., **Samios J**

***J. Chemical Physics*** *133*, 014504. **(2010**)

---

- "Adsorption of $N_2$, $CH_4$, CO and $CO_2$ gas in Single Walled Carbon Nanotubes: A Combined Experimental and Monte Carlo Molecular Simulation Study",

**G. P. Lithoxoos, A. Labropoulos, L. Peristeras, N. Kanellopoulos, J. Samios** and **I. G. Economou**

***J. Supercritical Fluids*** *55*, 510. **(2010)**

---

- "Solvation Structure and Dynamics of cis- and trans-1,2 Dichloroethene Isomers in Supercritical Carbon Dioxide. A Molecular Dynamics Simulation Study"

**D. Dellis, I. Skarmoutsos, J. Samios**

***J. Physical Chemistry B*** 115, 12098 (**2011)**

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- Quantitative study of diffusion jumps in atomistic simulations of model gas-polymer systems

**Raptis, Th. E., Raptis, V. E., Samios, J.**

***Molecular Physics*** 110, 1171 **(2012)**

---

- "Interaction between silicon-carbide nanotube and cholesterol domain. A Molecular dynamics simulation study"

**Raczynski P, Gorny K, Samios J , Gbourski Z,**

***J Physical Chemistry C,*** 118, 30115 **(2014)**

---

- "Molecular Dynamics study of the local structure and diffusivity of partially miscible water/n-alcohols binary mixtures"

**Dimitroulis C, kainourgakis E, Raptis V, Samios J.**

**Journal of Molecular Liquids,** 205, 46 **(2015)**

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- '' Dynamics and drift motion of $O_2^-$ in supercritical argon"

**Koutselos A. D, Samios J**

**Journal of Molecular Liquids,** 205, 115 **(2015)**

---

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

**Elpidoforou N, Dimitroulis C, Skarmoutsos I, Samios J.**

**Fluid Phase Equilibria,** Subm. Sept. (**2015**)

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