

CURRICULUM VITAE

2008

Dr. George E. Froudakis

Office address

Department of Chemistry, University of Crete
PO Box 2208, Voutes, Heraklion Crete, 710 03 GREECE

Tel: +302810 545055

Fax: +302810 545001

E-mail: frudakis@chemistry.uoc.gr

URL : <http://tccc.iesl.forth.gr/~frudaki>

PERSONAL

Date of Birth : October 24, 1968.

Place of Birth : Iraklion Crete, Greece.

Nationality : Greek.

EDUCATION

1986-1990 : Under-graduate studies in the Physics department of the University of Crete, Greece. **Diploma obtained in 1990.**

1990-1995 : Graduate studies in the Physics department of the University of Patras, Greece.
Advisor: Prof. A. D. Zdetsis. Part of the thesis made in the Institute of Physical and Theoretical Chemistry, University of Bonn, Germany, in collaboration with Prof. S. D. Peyerimhoff.

Ph.D. thesis : “Theoretical Investigation of Low Symmetry Semiconductor Systems, In Real Space”. **Ph.D. obtained in 1995.**

Languages : Greek, English.

WORKING EXPERIENCE

1997-2002: Visiting Professor in the Chemistry department of the University of Crete.

2002-2007 : Assistant Professor of Computational Chemistry in the Chemistry department of the University of Crete.

2207- : Associate Professor of Computational Chemistry in the Chemistry department of the University of Crete.

2007- : Member of directors of the Greek Hydrogen Platform.

Teaching experience

- 1990-1991: ‘Computational Physics’ seminars for graduate Physicists in University of Patras.
- 1997-2001: ‘Mathematics for Chemists I and II’, dept. of Chemistry, University of Crete.
- 1998-1999 & 2001-: ‘Computational Chemistry’, department of Chemistry, University of Crete.
- 1998-1999 & 2001-: ‘Quantum Chemistry’, department of Chemistry, University of Crete.
- 1998- : ‘Computational methods in Quantum Chemistry’, postgraduate, dept. of Chemistry, University of Crete.

Supervision of PhDs thesis

- G. Mpourmpakis “Theoretical study of hydrogen storage in Nanotubes” 2006

- A. Mavrantoukakis “Theoretical study of elementary chemical phenomena in biological systems with quantum and classical methods” 2006 (co-supervision with Prof. Farantos)
- E. Klontzas “Theoretical study of hydrogen storage in novel Nanomaterials” start in 2005
- G. Dimitrakakis “Theoretical study of atomic and molecular hydrogen interaction with carbon nanostructures” start in 2005
- A. Gotzias “Combination of experimental and theoretical multi-scale techniques for studying gas adsorption in nano-based and porous materials”, (co-supervision with Prof. D. Theodorou and Dr. T. Steriotis in collaboration with Democritus National Lab).

Supervision of MSc thesis

- G. Mpourmpakis “Theoretical study of transition metal encapsulation in Si clusters-formation of Nanotubes” 2003
- A. Mavrantoukakis “Theoretical study of Silicon – Carbon Nanotubes” 2005
- E. Klontzas “Theoretical study of hydrogen storage in Metal Organic Frameworks” start in 2005
- K. Vogiazis “ Theoretical study of CO₂ storage in novel Nanomaterials” start in 2006

GRANTS

- Greek - German Collaboration Program. Title: ‘*Ab-initio* Investigation of Silicon - Carbon Clusters’. (1992-98).
- Greek Scientific Program (ΙΙΕΝΕΔ). Title: ‘Atomic and Molecular Semiconductor and Metal Clusters’. (1993-95).
- Greek Scientific Program (*Karatheododis*). Title: ‘Theoretical investigation of low dimension semiconductor systems: Semiconductor clusters and Porous silicon’. (1998-2002).
- Greek Scientific and Educational Program (Ε.Π.Ε.Α.Ε.Κ.). Title: ‘Applied Molecular Spectroscopy’. (1998-).
- NATO Collaborative Linkage Grant. Title: ‘Studies of Elementary Steps of Radical Reactions in Atmospheric Chemistry’. (2000-02). (Co-PI). 24.600 \$
- Greek - Cyprus Collaboration Program. Title: ‘Studying the Anti-oxidized action of cancer related compounds’ (2000-2002)
- Greek - France Collaboration Program. Title: ‘Oxidized distraction of DNA by free radicals’ (2000-2002)
- Greek - German Collaboration Program.: (IKYDA 2000), Title: ‘Characterisation of selected Si-C and Si-Ge clusters by Quantum Chemistry methods’. (PI). 18.000 €

- Greek Scientific Program (*HRAKLEITOS*). Title: ‘Theoretical investigations of hydrogen storage in carbon nanotubes’ (2003-2006). (PI). 33.000 €
- Greek Scientific Program (*PYTHAGORAS*). Title ‘Novel energy storage materials: Theoretical investigation of hydrogen storage in carbon nanotubes and nanoscrolls’ (2003-2006). (PI). 80.000€
- Greek Scientific Program (*PYTHAGORAS II*). Title ‘Dynamics and reactivity of protein reactions: Spectroscopic and theoretical investigation’ (2005-2006). (Co-PI). 50.000€
- Greek Scientific Program (ΠΕΝΕΔ). Tile: ‘Hydrogen Storage in Nano-Materials for Fuel Cell Applications ’. (2005-2008). (PI). 190.000 €
- Greek - German Collaboration Program: (IKYDA 2005), Title: ‘A Multi-Scale theoretical study of hydrogen storage in Nano-Materials’. (2006-2007) (PI). 20.000 €
- INTERREG IIIA. title : ‘Training and research in nano-materials and nanotechnology: design, synthesis and applications’.(2006-2008) 305.000 €
- FP6 Integrated Project NESSHY title: Novel Efficient Solid Storage for H₂ (2006-2010)

RESEARCH AREAS

- Ab-initio investigation of structural and electronic properties, of organic and inorganic molecules.
- Large scale calculations of polymeric and biologically important systems with the use of ab-initio and semiempirical methods.
- Study of chemical reactions.
- Theoretical study of the electronic spectra of small molecules.
- Theoretical investigation of carbon Nanotubes. Study of the catalytic procedure and of metal encapsulation.
- Study of hydrogen adsorption in C-based materials and Metal Organic Frameworks.
- Theoretical investigation of amorphous materials surfaces and interfaces combining computational physic and quantum chemistry methods.

REVIEWER IN INTERNATIONAL SCIENTIFIC ORGANIZATIONS

- National Science Foundation (NSF) - USA
- Department of Energy (DOE) - USA

REVIEWER IN SCIENTIFIC JOURNALS

- Physical Review Letters (PRL)
- Journal of the American Chemical Society (JACS)

- Nano Letters (NL)
- Journal of Nanoscience and Nanotechnology (JNN)
- Physical Review B (PRB)
- Journal of Physical Chemistry - Chemical Physics (PCCP)
- Journal of Chemical Physics (JCP)
- Journal of Physical Chemistry (JPC)
- Chemical Physics Letters (CPL)
- International Journal of Quantum Chemistry

PUBLICATIONS

1. "Energetics and Structure of db and fb States in a-Si", A.Zdetsis and G.Froudakis, Journal of Non Crystalline Solids, 137, 303 (1991).
2. "Model Potential for Silicon Clusters and Surfaces" A.D.Mistriotis, G.E.Froudakis, P.Vendras, N.Flytzanis, Physical Review B47, 10648 (1993).
3. "Reproduction of Quantum Tight-Binding Effects in Silicon Clusters by a 4-Body Classical Model", A.D.Mistriotis, A.D. Zdetsis, G.E.Froudakis, M.Menon, Journal of Physics C5, 6183 (1993).
4. "Importance of multicenter bonding in the structure of Si_3C_3 ", M.Muhlhauser, G.Froudakis, A.Zdetsis, S.Peyerimhoff, Chemical Physics Letter 204 (1993) 617.
5. "Ab-initio investigation of the stability of Si_3C_3 clusters and their structural and bonding features" M.Muhlhauser, G.Froudakis, A.Zdetsis, B.Engels, S.Peyerimhoff, N.Flytzanis, Zeitschrift fur Physik D32, 113 (1994).
6. "A comparative ab-initio study of the Si_2C_4 , Si_3C_3 , Si_4C_2 clusters", G.Froudakis, A.Zdetsis, M.Muhlhauser, B.Engels, S.Peyerimhoff, Journal of Chemical Physics, 101 6790 (1994).
7. "Theoretical study of the Si_3C_2 cluster", G.Froudakis, M.Muhlhauser, A.Zdetsis, Chemical Physics Letter 233, 619 (1995).
8. "Ab initio study of electronic, structural and vibrational properties of the Si_4C cluster", A.Zdetsis, G.Froudakis, M.Muhlhauser, H.Thumnel, Journal of Chemical Physics, 104,2566 (1996).
9. "Binding energies and structures of C^+Ar_n ($n=1-5$), clusters from first principles", G.E.Froudakis, G.S.Fanourgakis, S.C.Farantos, S.S.Xantheas, Chem.Phys.Lett.294 (1998) 109.
10. "Stability and structure of Ni^+Ar_n and Pt^+Ar_n clusters", M.Velegrakis, G.E.Froudakis, S.C.Farantos, Journal of Chemical Physics (Letters), 109 (1998) 4687
11. "A tight-binding molecular dynamics study of Ni_mSi_n binary clusters", A.N.Andriotis, M.Menon, G.E.Froudakis, Z.Fthenakis, J.E.Lowther, Chem. Phys. Lett. 292 (1998) 487.

12. "Tight-Binding Molecular Dynamics study of Transition Metal Carbide Clusters", A.N.Andriotis, M.Menon, G.E.Froudakis, J.E.Lowther, Chem. Phys. Lett. 301(1999)503.
13. "Coordination of Ti cation embedded in Argon clusters", M.Velegakis, G.E.Froudakis, S.C.Farantos, Chem.Phys.Lett. 302 (1999) 595.
14. "Tight-Binding Molecular Dynamic study of Heteronuclear systems: Application on Si_mGe_n Clusters", A.Andriotis, M.Menon, G.Froudakis, Journal of Cluster Science, 10, (1999) 549.
15. "Complete assignment of ^1H - and ^{13}C - NMR spectra of Poly(N-vinylcarbazole)", A.Karali, G.Froudakis, P.Dais, Macromolecules 33 (2000) 3180.
16. "Curvature dependence of the metal catalyst atom interaction with carbon nanotube ", M.Menon, A.Andriotis, G.Froudakis, Chem. Phys. Lett. 320 (2000) 425.
17. "Anomalous temperature dependence of the resistivity of Single Wall Carbon Nanotubes ", A. Andriotis, M.Menon, G.Froudakis, Physical Review B. 61 (2000) 13393, Rapid Communication.
18. "Site Specificity in the Photo-oxidation of Some Trisubstituted Alkenes in Thionin-Supported Zeolite Na-Y. On the Role of Alkali Metal Cation", M.Stratakis, G.Froudakis, Organic Letters 2 (2000) 1369.
19. "Various bonding configurations of transition metal atoms on carbon nanotubes : Their effect on contact resistance", A.Andriotis, M.Menon, G.Froudakis, Applied Physics Letters 76(2000) 3890.
20. "The electronic spectrum of linear and rhombic C_4 ", M.Muhlhauser, G.Froudakis, M.Hanrath, S.Peyerimhoff, Chemical Physics Letters 324 (2000) 195.
21. "Contrasting bonding behaviors of 3-D transition metal atoms with graphite and C_{60} ", A.Andriotis, M.Menon, G.Froudakis, Phys. Rev. B, Brief Report, 62 (2000) 9867.
22. "Mass Spectra and Theoretical Modeling of Li^+Ne_n , Li^+Ar_n and Li^+Kr_n Clusters", G.E.Froudakis, S.C.Farantos, M.Velegakis, Chemical Physics 258 (2000) 13.
23. "Catalytic action of Ni atoms in the formation of Carbon Nanotubes: A molecular dynamics study", A.Andriotis, M.Menon, G.Froudakis, Physical Review Letters 85 (2000) 3193.
24. "cis- and trans- N-Benzyl-octahydrobenzo[g]quinolines. Adrenergic and Dopaminergic Activity Studies", K.Thermos, G.E.Froudakis, N.Tagmatarxis, X.Katerinopoulos, Bioorganic and Medicinal Chemistry Letters 11 (2001) 883.
25. "An MRD-CI Study of the Electronic Spectrum of Linear C_9 ", M.Muhlhauser, G.Froudakis, S.Peyerimhoff, Chemical Physics Letters 336 (2001) 171.
26. "Hydrogen Interaction with Single Wall Carbon Nanotubes. A Combined Quantum-Mechanics / Molecular-Mechanics study", G. E. Froudakis, Nano Letters 1 (2001) 179.

27. "Stereochemistry in the reaction of 4-methyl-1,2,4-triazoline-3,5-dione (MTAD) with β,β -dimethyl-p-methoxystyrene. Are open biradicals the reaction intermediates? ", M.Stratakis, M.Hatzimarinaki, G.Froudakis, M.Orfanopoulos, J. Org. Chem. 66 (2001) 3682.
28. "Theoretical and Experimental Studies of the Metallated Phenanthroline Derivatives. Optimization of the Nitrate Sensor", G.Andreadakis, E.Moschou, K.Matthaiou, G.Froudakis, N.Chaniotakis, Analytica Chimica Acta 439 (2001) 273.
29. "Ab initio CCSD(T) and MRD-CI study of excited states and the electronic spectrum of linear C5+", M. Schnell, M. Muhlhauser, G.E. Froudakis, S.D. Peyerimhoff, Chemical Physics Letters 340 (2001) 559.
30. "Structural Properties of Metal-Benzene, $M_n(\text{benzene})_m$, $M=\text{Ni}, \text{V}$, Complexes: An *ab-initio* study", G.E.Froudakis, A.Andriotis, M.Menon, Chemical Physics Letters 350 (2001) 393.
31. "Extreme hydrogen sensitivity of the transport properties of Single Wall Carbon Nanotubes", A.Andriotis, M.Menon, D.Srivastava, G.Froudakis, Physical Review B 64 (2001) 193401.
32. "Ground state geometry of small Ni-C clusters", G.E. Froudakis, M. Muhlhauser, A. Andriotis, M. Menon, Physical Review B64 (2001) 241401, Rapid Communication.
33. "The electronic spectrum of C₁₁ in its linear and cyclic conformation", M.Muhlhauser, G.Froudakis, S.Peyerimhoff, Phys. Chem. Chem. Phys. 3 (2001) 3913.
34. "Why alkali doped Carbon Nanotubes poses high hydrogen uptake", G. E. Froudakis, Nano Letters 1 (2001) 531.
35. "Structure and stability of Ni-encapsulated Si nanotubes", M. Menon, A. Andriotis, G.E. Froudakis, Nano Letters 2 (2002) 301.
36. "Importance of the multi-reference configuration interaction of the $^3\Sigma_u^- \leftarrow X^3\Sigma_g^-$ transitions of the linear HC₇H", G. Mpourmpakis, M.Muhlhauser, G.Froudakis, S.Peyerimhoff, Chemical Physics Letters 356 (2002) 398.
37. "Stereochemistry of the reaction of [4+2] cycloadditions of the trans, trans- and cis, trans-2,4-Hexadiene to C(60) ", N.Chronakis, G.Froudakis, M.Orfanopoulos, J. Org. Chem. 67 (2002) 3284.
38. "Mass Spectra and Structures of the Cu⁺Rg_n Clusters (Rg = Ne, Ar) ", G.E.Froudakis, M.Muhlhauser, S.C.Farantos, A.Sfounis, M.Velegarakis, Chemical Physics 280 (2002) 43.
39. "The electronic spectrum of linear Pentadiynylidene in comparison with isomeric Ethynylcyclopropylidene", A. Mavrandonakis, M.Muhlhauser, G.Froudakis, S.Peyerimhoff, Phys. Chem. Chem. Phys.4 (2002) 3318.
40. "Photofragmentation spectra of Sr⁺CO complex: experiment and ab-initio calculations", S.C.Farantos, E.Filippou, S.Stamatiadis, G.E.Froudakis, M.Muhlhauser, M.Masaouti, A.Sfounis, M.Velegarakis, Chem. Phys. Let. 366 (2002) 231-237.

41. "5-Endoring Radical Cyclizations: Disfavored or Favored Processes? ", C.Chatgialoglou, C.Ferreri, M.Guerra, V.Timokhin, G.E.Froudakis, T.Gimisis, submitted to J. American Chemical Society 124 (2002) 10765.
42. "Stabilization of Si-based cage clusters and nanotubes by encapsulating transition metal atoms", A. Andriotis, G. Mpourbakis, G.E. Froudakis, M. Menon, New J. Phys. 4 (2002) 78.
43. "A DFT study on the interaction of Li^+ and Na^+ to alkali-substituted ethens", G.Froudakis, M.Stratakis, Eur. J. Org. Chem. (2003) 359-364.
44. "Ene Hydroperoxidation of Isobutenylarenes within Dye-Exchanged Zeolite Na-Y: Control of Site Selectivity by Cation – Arene Interactions", M.Stratakis, C.Rabalakos, G.Mpourmpakis, G.Froudakis, J. Org. Chem. 68 (2003) 2839-2843.
45. "Pathways for Oxygen Adsorption on Single Wall Carbon Nanotubes", G.E. Froudakis, M. Schnell, M. Muhlhauser, S.Peyerimhoff, A. Andriotis, M. Menon, R.Sheetz, Physical Review B68 (2003) 115435.
46. "The excited states of Sr^+CO : Photofragmentation spectra and ab-initio calculations", S.C.Farantos, E.Filippou, S.Stamatiadis, G.E.Froudakis, M.Muhlhauser, M.Peric, M.Masaouti, A.Sfounis, M.Velegakis, Chem. Phys. Let. 379 (2003) 242-247.
47. "From Pure Carbon to Silicon Carbon Nanotubes. An ab-initio Study", A.Mavrantonakis, G.E. Froudakis, M. Schnell, M. Muhlhauser, NanoLetters 3 (2003) 1481-1484.
48. "Understanding the structure of metal encapsulated Si cages and nanotubes: The interplay of symmetry and d-band filling", G. Mpourbakis, G.E. Froudakis, A. Andriotis, M. Menon, J. Chem Phys. 119 (2003) 7498-7502.
49. "Fe encapsulation by silicon clusters: Ab-initio electronic structure calculations", G. Mpourbakis, G.E. Froudakis, A. Andriotis, M. Menon, Phys. Rev. B 68 (2003) 125407.
50. "Ab-initio MRDCI investigation of liner HC_5H^+ and HC_7H^+ ", M.Muhlhauser, J.Haubrich, G. Mpourmpakis, A. Mavrantonakis, G.Froudakis, El. J. Mol. Des. 1 (2003) 578.
51. "Structure and Stability of SiC Nanotubes", M. Menon, E.Richter, A.Mavrantonakis, G.E. Froudakis, A. Andriotis, Phys. Rev. B 69, (2004) 115322.
52. "An MRD-CI study of the electronic spectrum of Si_3C_3 ", M.Muhlhauser, G.Froudakis, A.Zdetsis, J. Mol. Spectroscopy 223 (2004) 96-100.
53. "Magnetic enhancement and magnetic reduction in binary clusters of transition metal atoms", A. Andriotis, G. Mpourmpakis, G.E. Froudakis, M. Menon, J. Chem. Phys 120 (2004) 11901.
54. "State-specific RKKY interaction in small magnetic clusters", A. Andriotis, G. Mpourmpakis, G.E. Froudakis, M. Menon, Phys. Rev. B. 70 (2004) 104421.
55. "The role of Co in enhancing the magnetism of small Fe clusters", G. Mpourmpakis, G.E. Froudakis, A. Andriotis, M. Menon, Phys. Rev. B. 72 (2005) 104417 .

56. "Carbon-Nanotube Tips with edge made of a transition metal", G. Mpourmpakis, G.E. Froudakis, A. Andriotis, M. Menon, Applied Physics Letters 87 (2005) 193105.
57. "Hydrogen Storage in Carbon Nanotubes. A Multi-scale Theoretical Study" G. Mpourmpakis, E. Tylianakis G.E. Froudakis, J. Nanoscience & Nanotechnology. 6 (2006) 87.
58. "Glycine interaction with carbon nanotubes: An ab-initio study" Mavrandonakis A, Farantos SC, Froudakis GE, J Phys Chem B 110 (2006) 6048.
59. "SiC nanotubes: A novel material for hydrogen storage" Mpourmpakis G, Froudakis GE, Lithoxoos GP, Samios J. Nano Letters 6 (2006) 1581.
60. "Silicon carbide nanotube tips: Promising materials for atomic force microscopy and/or scanning tunneling microscopy" Mavrandonakis A, Froudakis GE, Andriotis A, Menon M, Applied Physics Letters 89 (2006) 123126.
61. "A Multi Scale Theoretical Study of Li⁺ Interaction with Carbon Nanotubes" G. Mpourmpakis, E. Tylianakis, D. Papanikolaou, G. E. Froudakis, J. Nanosci. Nanotechnol. 6, 3731-3735 (2006)
62. "Why alkali metals preferably bind on structural defects of carbon nanotubes: A theoretical study by first principles," G. Mpourmpakis and G Froudakis, Journal of Chemical Physics 125, 204707 (2006).
63. "Haeckelites: A promising anode material for lithium batteries application. An ab initio and molecular dynamics theoretical study", G. Mpourmpakis, G. E. Froudakis, E. Tylianakis, Applied Physics Letters 89, 233125 (2006)
64. "Why boron nitride nanotubes are preferable to carbon nanotubes for hydrogen storage? An ab initio theoretical study" G. Mpourmpakis, G. E. Froudakis, Catalysis Today, 120, 341-345 (2007).
65. "The Effect of Curvature and Chirality for Hydrogen Storage in SWNTs. A Combined Ab-initio and Monte-Carlo Investigation." Mpourmpakis G, Froudakis GE, Lithoxoos GP, Samios J., J. Chem. Phys. 126, 144704 (2007).
66. "Enhancement of the ionization-potential of K and Rb upon chemisorption on a C60 molecule", G. Mpourmpakis, G.E. Froudakis, A. Andriotis, M. Menon, J. Phys. Chem. C, Accepted (2007)
67. "Carbon Nanoscrolls: A Promising Material for Hydrogen Storage" G. Mpourmpakis, E. Tylianakis and G.E. Froudakis, NANO LETT 7 (2007) 1893-1897.

→ "Roll up for better hydrogen fuel storage" –

25 June 2007 – Special report in New Scientist ←

68. "Molecular Hydrogen Interaction with IRMOF-1: A Multiscale Theoretical Study" E. Klontzas, A. Mavrandonakis, G.E Froudakis, Y. Carissan, W. Klopffer, J. Phys. Chem. C 111(2007) 13635-13640.

69. "Assessing the Density Functional Theory in the Hydrogen Storage Problem", G. Mpourmpakis and G. E. Froudakis, J. Nanosci. Nanotechnol. (2007) Accepted.
70. "Why Li doping in MOFs enhances H₂ storage capacity? A multi-scale theoretical study." A. Mavrandonakis, E. Tylianakis, A.K. Stubos and G.E. Froudakis, J. Phys. Chem. C, Accepted (2008)
71. "Hydrogen Storage in 3-D COFs. A multi-scale theoretical investigation." E. Klontzas, E. Tylianakis, G. E. Froudakis, Phys. Chem. C, Accepted (2008)

Invited Review Articles

1. "Hydrogen Interaction with Carbon Nanotubes. A Review of ab-initio studies", G. E. Froudakis, Journal of Physics – Condensed Matter 14 (2002) 453.
2. "Hydrogen and Oxygen Interaction with Carbon Nanotubes", G. E. Froudakis, Encyclopedia of Nanoscience and Nanotechnology (2003) v4, p1-11; **"2005 Best Reference Work Award"** from the American Society of Engineering Education.
3. "Hydrogen Storage in SWNTs. A Mixed QM/MM study", G. E. Froudakis, Review on Advanced Materials Science 5 (2003) 259.
4. "Theoretical modeling of the glycine radical addition to carbon Nanotubes" Mavrandonakis A, Farantos SC, Froudakis GE Review on Advanced Materials Science 11 (2006) 88.
5. "Theoretical study of alkaline metal cations in carbon Nanotubes" Mpourmpakis G, Tylianakis E, Papanikolaou D, Froudakis G.E. Review on Advanced Materials Science 11 (2006) 92.
6. Chapter in Book: "Chemistry of Carbon Nanotubes" (V.A. Basiuk and E.V. Basiuk, Eds.). by American Scientific Publishers, Title: Interaction of hydrogen with carbon Nanotubes, G. Mpourmpakis, E. Tylianakis, G. E. Froudakis,

INVITED TALKS

- University of Barcelona, Spain, Department of Physical Chemistry, July 2, 1998.
Title: "Binding energies and structures of C⁺Ar_n (n=1-5), clusters from first principles"
- University of Ioannina, Greece, Department of Chemistry, December 17, 1999.
Title: 'Theoretical calculations for the structural and electronic properties of molecules.'
- University of Patras, Greece, Department of Physics December 20, 1999.
Title: 'Quantum chemistry calculations in clusters'.
- University of Bonn, Institute of Physical and Theoretical Chemistry, February 10, 2000.
Title: "Inert Gas Atomic Clusters Doped by Various Metal and Non-Metal Cations. Applications on C⁺ and Li⁺."

- Technical University of Crete, Greece, March 24, 2000.
Title: 'Quantum chemistry calculations in clusters: Application in the study of new materials'.
- University of Kentucky, Department of Physics, April 18, 2000.
Title: "Ab-initio investigation of Cation Doped, Inert Gas Atomic Clusters"
- University of Patras, Greece, Department of Physics, September 15, 1999.
Title: 'Quantum chemistry calculations in clusters. Application in the study of carbon nanotubes'.
- 1st Workshop on Collaborative Actions in Computational Materials Science, October 03, 2000, Heraklion.
Title: 'Molecular Quantum Chemistry Calculations in Materials Science: Application on Single Walled Carbon Nanotubes'.
- University of Cyprus, Dept. of Chemistry, October 23, 2000.
Title: 'Quantum Chemical Molecular Calculations in Materials: Application on Carbon Nanotubes.'
- IESL-Forth Colloquium, May 23, 2001 Crete.
Title: 'Molecular Quantum Chemistry Calculations in Materials Science: Application on Carbon Nanotubes'.
- Institute of Physical and Theoretical Chemistry, University of Bonn, July 2001.
Title: 'Molecular Quantum Chemistry Calculations in Materials Science: Application on Carbon Nanotubes'.
- 2nd Workshop on Synthesis and Characterization of Nanostructured Materials, October 2001, Heraklion
Title: 'Why Alkali Doped Carbon Nanotubes Posses High Hydrogen Uptake?'
- Physics Dept. Colloquium, February 21, 2002 Crete.
Title: 'Molecular Quantum Chemistry Calculations in Materials Science: Application on Carbon Nanotubes'.
- University of Crete, Dept. of Physics, Lecture on 'Modern Physics Lectures', March 2002
Title: 'Nanotechnology'
- 3rd Workshop on Synthesis and Characterization of Nanostructured Materials, Sept. 2002, Heraklion.
Title: 'Atomic and Molecular Oxygen Adsorption on Carbon Nanotubes'
- Center for Computational Sciences – University of Kentucky –Fall Wednesday Seminars, Nov.19 2003.
Title: 'Hydrogen and Oxygen Interaction with Carbon Nanotubes'
- International Conference on Computational & Experimental Engineering and Sciences, Madeira,2004
Title: 'Hydrogen Storage on Nanotubes and Nanoscrolls'
- University of Crete- Physics Dept., 17th Summer School of Advanced Computational Physics, 2005.
Τίτλος: 'Nano-CAD : Computer Aided Nano-material Design'.
- IPHE International Hydrogen Storage Technology Conference Lucca Italy 19-22 June 2005

Title: 'Theoretical study of Hydrogen Storage in Nanotubes and Nanoscrolls'

- International Conference on ENERGY, ENVIRONMENT, ECOSYSTEMS and SUSTAINABLE DEVELOPMENT, Athens, July 12-14, 2005

Title: 'Hydrogen Storage in SWNT. A Combined Ab-initio and Molecular Mechanics – Molecular Dynamics Investigation'

- 20th Greek Conference on Chemistry, September 2005 Ioannina.

Title: 'Theoretical study of Hydrogen Storage in Nanotubes'

- Department of Chemistry, University of Karlsruhe, Germany, November 2005

Title: 'NanoCAD - Computer Aided Nonmaterial Design'

- International Korean Conference on Innovative Science and Technology (KCIT-2005) December 4-7, 2005, Gyeongju, Korea.

Title: 'Theoretical investigation of hydrogen storage in Nanotubes'

- Rutherford Appleton Laboratory UK, ISIS colloquium, 23rd Jan. 2007,

Title: "Designing Nanoporous Materials for Hydrogen Storage"

- University of Calabria, department of Physics, colloquium, October 10th, 2007,

Title: "Designing Novel Nanoporous Materials for Hydrogen Storage"

- Department of Chemistry, University of Crete, December 2007

Title: "Designing Novel Nano-Materials for Hydrogen Storage"

PARTICIPATION IN SCIENTIFIC MEETINGS

1. 14th International Conference of Amorphous Semiconductors August '91 in Garmish-Partenkirchen, Germany.
2. VII Hellenic Conference in Solid State Physics, September '91 in Thessaloniki, Greece.
3. 1st Conference of the Balcan Physics Union September '91 in Thessaloniki, Greece.
4. NATO ASI¹ "Localisation and Propagation of Classical Waves in Random and Periodic Structures" May '91 in Agia Pelagia, Greece.
5. NATO ASI¹ "Statics and Dynamics of Alloy Phase Transformations", June '92 Rhodes, Greece.
6. VIII Hellenic Conference in Solid State Physics, September '92 in Ioannina, Greece.
7. IX Hellenic Conference in Solid State Physics, September '93 in Patras, Greece.
8. X Hellenic Conference in Solid State Physics, September '94 in Delfoi, Greece.
9. NATO ASI¹ "Stability of Materials", June '95, in Corfu, Greece.
10. NATO ASI¹ "Actinides and Environment" July '96, Maleme, Greece.
11. XII Hellenic Conference in Solid State Physics, September '96 in Heraklion, Greece.

12. NATO ASI¹ "Hydrogen Bonding", June 1997, Eluda – Crete.
13. XIV Hellenic Conference in Solid State Physics, September '98 in Ioanina, Greece
14. 5th Patras Euroconference on "Bulk Magnetic and Superconducting Novel Materials"
15. September 1998, Patras, Greece. "Wave Propagation and Electronic Structure in Disordered Systems", June 15, 2000, Heraklion, Greece.
16. XVI Hellenic Conference in Solid State Physics, September 2000, Nafplion, Greece.
17. 1st Workshop on Collaborative Actions in Computational Materials Science, October 03, 2000, Heraklion, Greece.
18. First Conference on Microelectronics, Microsystems and Nanotechnology, 20-22 November 2000, Athens, Greece.
19. 1st Workshop on Collaborative Actions in the Study of Atmospheric Chemistry, December 4 2000, Heraklion, Greece.
20. CECAM-SIMU workshop on Multiscale Modeling of Materials. Methods, Algorithms and Unsolved Problems. July 2001, Greece.
21. 2nd Workshop on Synthesis and Characterization of Nanostructured Materials, October 2001, Heraklion.
22. 3rd Workshop on Collaborative Actions in the Study of Atmospheric Chemistry, May 2002, Ioanina, Greece.
23. 3rd Workshop on Synthesis and Characterization of Nanostructured Materials, Sept. 2002, Heraklion.
24. XVIII Hellenic Conference in Solid State Physics and Materials Science, September 2002 Heraklion, Greece
25. 19^o Greek Conference on Chemistry, November 2002, Heraklion, Greece.
26. Nanomaterials and Nanotechnology NN2003, August 2003, Crete.
27. International Conference on Computational & Experimental Engineering and Sciences, Madeira, July 2004.
28. XX Hellenic Conference in Solid State Physics and Materials Science, September 2004 in Ioanina, Greece. ***Best oral presentation award.***
29. 1st Greek conference on Hydrogen Technologies, September 2004, Athens
30. Nanomaterials and Nanotechnology NN2003, June 2005, Crete
31. IPHE International Hydrogen Storage Technology Conference 19-22 June 2005, Lucca, Italy.
32. International Conference on ENERGY, ENVIRONMENT, ECOSYSTEMS and SUSTAINABLE DEVELOPMENT, Athens, July 12-14.
33. 20th Greek Conference on Chemistry, September 2005, Ioannina.
34. 2nd Greek Symposium of Porous materials, September 2005, Democritus.
35. 2nd Greek conference on Hydrogen Technologies, October 2005, Thessalonica
36. International Korean Conference on Innovative Science and Technology

(KCIT-2005) December 4-7, 2005, Gyeongju, Korea.

37. U.S. Department of Energy, Hydrogen Annual Meeting, Theory Focus Session on Hydrogen Storage Materials, Washington D. C. May, 16-19, 2006
38. International Conference of Computational Methods in Sciences and Engineering, Chania 27/10-1/11 2006.
39. 3rd Greek Symposium of Porous materials, October 2007, Thessaloniki.
40. 3rd Greek conference on Hydrogen Technologies, October 2007, Patras