Zacharias G. Fthenakis

Research Associate

Istituto Nanoscienze Consiglio Nazionale Delle Ricerche (CNR-NANO),

Phone number website

e-mail

1. CURRICULUM VITAE

:

<u>Personal</u> <u>Information</u>	Date and Place of birth:Marital status:Military service:Nationality:Languages:	
<u>Education</u>	 Ph.D. Computational Condensed Mater Physics University of Crete, Heraklion, Greece Thesis: Study of Structural, Electronic, Thermodynamic and Magnetic properties of clusters using the Tight Binding Molecular Dynamics Method Supervisor: A.N.Andriotis 	May 2010
	M.Sc Condensed Matter Physics University of Crete, Heraklion, Greece	Sept. 1996
	B.Sc. in Physics University of Crete, Heraklion, Greece grade: 7.97/10 (Upper Second-Class Honours "II.1")	Nov. 1994
<u>Research</u> <u>Interests</u>	Modeling for the study of materials properties New Carbon allotropes, either 3-dimensional or 2-dimensional Ferroelectric materials Graphene, carbon nanotubes, fullerene-like structures and other materials Structural, thermodynamic, transport, magnetic and mechanical properties Magnetic properties of Dilute Magnetic Semiconductors Global Optimization Algorithms Human body composition	
<u>Awards</u>	Competition of the Hellenic Mathematical Society Summer School of Advanced Physics. Univ. of Crete	1988 1993

28/01/2024

IOP Trusted Reviewer

2020

<u>Scholarships</u>	 Successive full scholarships awarded from the Physics Department of the University of Crete and the Institute of Electronic Structure and Laser of the Foundation for Research and Technology, Hellas. EU TMR network "USEFULL" (Chemistry Department of the University of Exeter – U.K. (Prof. P.W.Fowler)) (June - August 2001) 	
<u>Employment</u>	 Instructor - Adjunct Professor - Visiting Assistant Professor Hellenic Mediterranean University, Greece 2000 - 2011 and (former Technological Educational Institute (TEI) of Crete) Fall 2013 - 2016 School of Pedagogical & Technological Education (ASPAITE), Greece University of West Attica, Greece Feb. 2020 - Sept.2021 	
	Research AssociateJune – Aug. 2001• University of Exeter, UKSupervisor: Prof. P. W. Fowler	
	 Postdoctoral Research Associate Michigan State University, MI, USA Supervisor: Prof. D. Tománek Sept. 2011 – Sept. 2013 Foundation for Research and Technology (FORTH), Greece Supervisor: Dr. A. N. Andriotis Jan. 2014 – Jan. 2015 University of South Florida, Tampa, FL, USA Supervisor: Prof. I. Ponomareva Jan. 2017 – May 2019 National Hellenic Research Foundation (NHRF), Greece Supervisor: Dr. N. N. Lathiotakis Sept. 2019 – Feb. 2021 Instituto Nanoscienze Consiglio Nazionale delle Ricerche (CNRnano), Italy Supervisor: Dr. V. Tozzini 	
Participation <u>in scientific</u> projects	 EU-GROWTH AM-MARE G5RD-CT-2001-00478 (FORTH, Greece) EU-TMR Network "USEFULL" (University of Exeter, UK) ARCHIMEDES II (TEI of Crete, Greece) NSF Cooperative Agreement no. EEC-0832785, (Michigan State University, USA) THALES code MIS: 380252 (FORTH, Greece) ARCHIMEDES III (MIS: 380353) (TEI of Crete, Greece) DOE Grant no. DE-SC0005254 (University of South Florida, USA) FLAG-ERA_"GATES" JTC-PCI2018-093137 (NHRF, Greece) MONSTRE-2D PRIN2017 KFMJ8E (IN-CNR, Italy) LESGO EU H2020-EIC-FETPROACT 2019-2020 (agreement no. 952068) (IN-CNR, Italy) 	
<u>Professional</u> (<u>teaching)</u> Experience	 A. <u>Teaching assistant</u> Department of Physics, University of Crete, Greece <u>Courses:</u> General Physics I (1 semester) Computers I (5 semesters) Computers II (3 semesters) Computational Physics I (1 semester) Computational Physics II (1 semester) Introduction to Solid State Physics (2 semesters) 	

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B. Instructor - Adjunct Professor - Visiting Assistant Professor

	2000 - 2002, 2000	3 - 2011, 2013 - 2016
Ca	ourses in Department of Human Nutrition and Dietet	tics:
◆]	Physics, Informatics I	2000 - 2001
♦]	Food and Radioactivity, Informatics III	fall 2001 – 2002
♦]	Informatics III	spring 2001 – 2002
♦]	Physics	2003 - 2004
♦]	Physics, Informatics I	2004 - 2005
♦]	Physics	2005 - 2006
♦]	Preparation and Presentation of Scientific Research,	
]	Principles of Physics. Physics Applications - Human	
]	Body Composition. Physics	2006 - 2007
♦]	Physics Applications - Human Body Composition.	
]	Informatics I, Principles of Physics	2007 - 2008
♦]	Physics Applications - Human Body Composition,	
]	Informatics II. Principles of Physics	2008 - 2009
♦]	Physics Applications - Human Body Composition.	
]	Principles of Physics, Biomathematics	2009 - 2010
♦]	Physics Applications - Human Body Composition.	
	Principles of Physics	2010 - 2011
♦]	Principles of Physics	fall 2013 – 2014
↓	Human Body Composition	spring 2014 – 2015
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C a	ourses in Department of Electrical Engineering:	
•	Electronics I	2001 - 2002
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<u>Co</u>	ourses in Department of Agricultural Technology:	
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◆ 1	Physics	fall 2014 – 2015
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1. Hellenic Mediterranean University, Greece

Courses in Department of Electrical and Electronic Engineering:

- Electrical Circuits I
- Electrotechnics and Electronic Technology

C. Other teaching experience

2000 - 2007

fall 2020 - 2021 spring 2020 – 2021

Institutes of Vocational Training, Crete, Greece **Teaching Physics and Informatics**

<u>Mentoring</u>	<u> Undergraduate thesis advisor – Hellenic Mediterranean University, Greece</u>
and	1. Dimitra Mpalaska
<u>supervision</u>	2. Iliopoulos Sotiris
of students	3. Giakoumaki Irini
	Michigan State University, USA
	1. Zhen Zhu (PhD thesis – 2015)
	2. Jie Guan (PhD thesis – 2017)
	University of South Florida, USA
	1 Maggie Kingsland PhD student
	2 Devin Pannas Master student
	3 Charles Montzer Undergaduate student
	A Kelli App I ynch Undergraduate student
	4. Keni Ann Lynch, Ondergraddale student
Editor	<i>Crystals</i> (Guest Editor for a special issue on the topic " <i>Density functional theory on</i>
Luitor	two-dimensional materials")
Referee in ≈ 40	• IOP Trusted Reviewer (awarded 2020)
Scientific	Energy & Environmental Science (39.714)
journals	Nature Communications (17.694)
(impact factor	Nano Letters (13.779)
in parenthesis)	• Carbon (11.307)
1	• ACS Applied Materials & Interfaces (10.383)
	• Physical Review Letters (9.161)
	• Nanoscale (8.307)
	Advanced Electronic Materials (7.633)
	• 2D Materials (6.861)
	Advanced Materials Interfaces (6.389)
	• Journal of Allovs and Compounds (6.371)
	• ChemComm (6.222)
	• ACS Applied Nanomaterials (6.14)
	• Frontiers in Chemistry (5.545)
	• Scientific Reports (4.997)
	• Molecules (4.927)
	• Journal of Chemical Physics (4.304)
	• ACS Omega (4.132)
	• RSC Advances (4.036)
	• Nanotechnology (3.953)
	• Applied Physics Letters (3.940)
	• Physical Review B (3.908)
	• Diamond and related materials (3.806)
	• Physical Chemistry – Chemical Physics (3.676)
	Computational Materials Science (3.572)
	• Journal of Physics D: Applied Physics (3.409)
	Physica Status Solidi – Rapid Research Letters (3.277)
1 1	The Journal of Physical Chemistry

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	 Superlattices and Microstructures (3.220) Inorganics (3.149) Physica Scripta (3.081) Physica B (2.988) Physical Review A (2.971) Journal of Physics: Condensed Matter (2.745) Chemical Physics (2.552) Journal of Applied Physics (2.286) Materials Research Express (2.025) Key Engineering Materials (0.350) Micro (not yet received)
<u>Computing</u> <u>Skills</u>	 Programming languages: Fortran (I have written several codes, mainly for molecular dynamics simulations based on the tight binding approximation and classic potentials) Experience with High Performance Computing Operating Systems: Unix/Linux, MS Windows Scientific packages: Siesta, VASP, Quantum Espresso, Gaussian, Materials Studio, LAMMPS, Gammes, Yaehmop, atom, etc Other useful software: Latex, Xfig, Office, Xmakemol, Xcrysden, Gnuplot, Xmgrace, etc
Development of scientific computational codes and algorithms (the codes are available upon request or they can be found here)	 Generation and enumeration of graphene pores with fixed number of 2-fold coordinated carbon atoms in the pore boundary (see <i>Carbon</i> 199, 508 (2022)) Construction of graphene pore structures using the nomenclature scheme proposed in <i>Carbon</i> 199, 508 (2022) Generation and enumeration of graphene pores, flakes and (periodic) edges with fixed number of 2-fold coordinated carbon atoms in their boundary. (Generalization of the code for pores, see <i>Nanomaterials</i> 13, 2343, (2023)) Construction of graphene flakes and (periodic) edges using the nomenclature scheme proposed in <i>Carbon</i> 199, 508 (2022). (Generalization of the code for pores, see <i>Nanomaterials</i> 13, 2343, (2023)) Construction of graphene flakes and (periodic) edges using the nomenclature scheme proposed in <i>Carbon</i> 199, 508 (2022). (Generalization of the code for pores, see <i>Nanomaterials</i> 13, 2343, (2023)) Calculation of the electronic structure of any crystal using the Harrisson's tight binding scheme Molecular dynamics code using either a tight binding Hamiltonian or classical potentials Calculation of (i) the rehybridized orbitals in non-planar sp² structures (ii) the tight binding Hamiltonian matrix elements for those orbitals using Papaconstantopoulos scheme, (iii) the contribution of each of those orbitals to the energy and (iv) the electronic structure of crystals based on the rehybridized orbitals Energy and force calculations of 10 classical potentials for transition metal systems (clusters or bulk structures) used in molecular dynamics and Monte Carlo simulations. The code also calculates force contributions from each atom for thermal conductivity calculations using the non-equilibrium molecular dynamics method. Phonon band structure calculation using the frozen phonon method. The code may calculate directly the forces of a classical potential if the appropriate both for molecules or extended systems.

25/01/2024

	 A multiple histogram method code for calculations of thermodynamic quantities obtained using molecular dynamics or Monte Carlo simulations. Improvement of the effective Hamiltonian molecular dynamics code, which is used for simulations of ferroelectric materials, to include interactions from antiferrodistortive local modes. Calculation of the pseudomagnetic ans pseudoelectric field in distorted graphene structures
<u>Schools</u>	 1992 : Summer School of Advanced Physics. Univ. of Crete, Greece 1993 : Summer School of Advanced Physics. Univ. of Crete, Greece 1994 : Summer School of Advanced Physics. Univ. of Crete, Greece 2021 : Bridging first Principal Calculations and Effective Hamiltonians. Hosted by Italian Institute of Technology, Genova, Italy (June 7 - 16)
<u>Current</u> <u>Collaborators</u>	 Dr. V. Tozzini, Instituto Nanoscienze Consiglio Nazionale Delle Ricerche (CNRnano), Italy Prof. I. Ponomareva, Physics Department, University of South Florida, Tampa, FL, USA Dr. A. N. Andriotis, Institute of Electronic Structure and Laser, Heraklion, Crete, Greece Dr. M. Menon, Department of Physics and Astronomy, University of Kentuky, Lexington, KY, USA Dr. N. N. Lathiotakis, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece Prof. D. Tománek, Physics and Astronomy Department, Michigan State University, East Lansing, MI, USA Prof. G. Kalosakas, Department of Materials Science, University of Patras, Patras, Greece Prof. B. Narayanan, Department of Mechanical Engineering, University of Louisville, USA Prof. V. Zafiropulos, Hellenic Mediterranean University, Greece
<u>Former</u> <u>Collaborators</u>	 Prof. P. W. Fowler, Department of Chemistry, University of Sheffield, Sheffield, UK Prof. G. Seifert, Physikalishe Chemie, Technische Universitat Dresden, Dresden, Germany Dr. R. W. A. Havenith, Zernike Institute for Advanced Materials, Groningen, The Netherlands Dr. A. Lappas, Institute of Electronic Structure and Laser, Heraklion,

Crete, Greece

28/01/2024

2. LIST OF PUBLICATIONS

<u>Refereed articles in international journals</u>

- 1. "Graphene membranes for gas separation" (**Z. G. Fthenakis**, N. N. Lathiotakis and I. D. Petsalakis) (submitted 2024)
- "Unusual phase transition mechanism induced by shear strain in Si₂BN planar structures and comparison with graphene: an ab-initio DFT study", Z. G. Fthenakis and M. Menon (submitted PRL - 2024)
- 3. "A generalized nomenclature scheme for graphene pores, flakes, and edges, and an algorithm for their generation and numbering", Z. G. Fthenakis, Nanomaterials 13, 2343 (2023)
- 4. "Evaluating the performance of ReaxFF potentials for sp² carbon systems (graphene, carbon nanotubes, fullerenes) and proposing a new ReaxFF potential", Z. G. Fthenakis, I. D. Petsalakis, V. Tozzini and N. N. Lathiotakis, Front. Chem. 10, 951262 (2022)
- 5. "A proposed nomenclature for graphene pores: a systematic study of their geometrical features and an algorithm for their generation and enumeration", Z. G. Fthenakis, Carbon 199, 508 (2022)
- 6. "Gas separation utilizing graphene membranes: a theoretical study" Z. G. Fthenakis, A. Fountoulakis, I. D. Petsalakis and N. N. Lathiotakis, Adv. Mater. Lett. 13, 031700 (2022)
- "High temperature stability, metalic character and bonding of Si₂BN planar structure" Z. G. Fthenakis, M. Jaishi, B. Narayanan, A. N. Andriotis and M. Menon, J. Phys. Cond. Matter 33, 165001 (2021)
- "The role of depolarization in the polarization reversal in ferroelectrics" M. Kingsland^{*}, Z. G. Fthenakis^{*} and I. Ponomareva, Phys. Rev. B 100, 024114 (2019) (^{*}equal contribution between these authors)
- "Structural deformations and mechanical properties of Si₂BN under uniaxial and uniform biaxial strain in comparison with graphene: An ab-initio study" Z. G. Fthenakis and M. Menon, Phys. Rev. B 99, 205302 (2019)
- 10. "Phase evolution in $BaTi_{1,x}Zr_xO_3$ ferroelectric relaxor from atomistic simulations" C. Mentzer, S. Lisenkov, Z. G. Fthenakis and I. Ponomareva, Phys. Rev. B 99, 064111 (2019)
- 11. "Intrinsic dynamics of electric-field-induced phase switching in antiferroelectric PbZrO₃ ultrathin films" Z. G. Fthenakis and I. Ponomareva, Phys. Rev. B **98**, 054107 (2018)
- 12. "All-mechanical polarization control and anomalous (electro)mechanical responses in ferroelectric nanowires" D. Pappas, Z. G. Fthenakis and I. Ponomareva, Nano Lett. 18, 5996 (2018)
- 13. "A torsional potential for graphene derived from fitting to DFT results" G. D. Chatzidakis, G. Kalosakas, Z. G. Fthenakis, K. Papagelis, N. N. Lathiotakis, Eur. Phys. J. B 91, 11 (2018)
- 14. "Dynamics of antiferroelectric phase transition in PbZrO₃", Z. G. Fthenakis and I. Ponomareva, Phys. Rev. B 96, 184110 (2017)
- 15. "Atomistic potential for graphene and other sp² carbon systems" Z. G Fthenakis, G. Kalosakas, G. D. Chatzidakis, C. Galiotis, K. Papagelis and N. N. Lathiotakis Phys. Chem. Chem. Phys. 19, 30925 (2017)
- 16. "Structural deformations of two dimensional planar structures under uniaxial strain: The case of graphene", Z. G. Fthenakis and N. N. Lathiotakis, J. Phys.: Cond. Matter 29,

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Zacharias G. Fthenakis - CV

175401 (2017) [This paper was highlighted as being particularly significant to the scientific community and is featured on <u>JPhys+</u> blog.]

- 17. "Are the experimentally observed 3-dimensional Carbon honeycombs, all-sp² structures? The dangling p-orbital instability." **Z. G. Fthenakis,** RSC Adv. **7**, 9790 (2017)
- 18. "Ab-initio investigation on the stability of H-6 Carbon", Z. G. Fthenakis, RSC Adv. 6, 78187 (2016)
- 19. "Electronic structure and transport in graphene/haeckelite hybrids: An ab-initio study" Z. Zhu, Z. G. Fthenakis and D. Tománek, 2D Materials 2, 035001 (2015)
- 20. "Graphene allotropes under extreme uniaxial strain: An ab-initio theoretical study" Z. G. Fthenakis and N. N. Lathiotakis, Phys. Chem. Chem. Phys. 17, 16418 (2015)
- 21. "Successive spin polarizations underlying a new magnetic coupling contribution in diluted magnetic semiconductors" A. N. Andriotis, Z. G. Fthenakis and M. Menon, J. Phys.: Cond. Matt. 27, 052202, (2015) (accepted as Fast Track Communication)
- 22. "Effect of structural defects on the thermal conductivity of graphene: From point to line defect to haeckelites" Z. G. Fthenakis, Z. Zhu, and D. Tománek, Phys. Rev. B 89, 125421 (2014)
- 23. "Topologically protected conduction state at carbon foam surfaces: An ab-initio study" Z. Zhu, Z. G. Fthenakis, J. Guan, and D. Tománek, Phys. Rev. Lett. 112, 026803 (2014)
- 24. "Limits of mechanical energy storage and structural transformations in twisted nanotube ropes" Z. G. Fthenakis, Z. Zhu, D. Teich, G. Seifert, and D. Tománek, Phys. Rev. B 88, 245402 (2013)
- 25. "Energetics of graphene flakes" Z. G. Fthenakis, Mol. Phys. 111, 3289 (2013)
- 26. "Nanomechanical energy storage in twisted nanotube ropes" D. Teich, Z. G. Fthenakis, G. Seifert, and D. Tománek, Phys. Rev. Lett. 109, 255501 (2012)
- 27. "Computational study of the thermal conductivity in defective carbon nanostructures" Z.
 G. Fthenakis, and D. Tománek, Phys. Rev. B 86, 125418 (2012)
- 28. "Uncovering the FURTEX-6100XL prediction equation for the percent body fat" Z. G. Fthenakis, D. Balaska, and V. Zafiropulos, J. Med. Eng. Technol. 36, 351 (2012)
- 29. "Structural and electronic properties of the fullerene isomers of Si₃₈: A systematic theoretical study" Z. G. Fthenakis, R. W. A. Havenith, M. Menon, and P. W. Fowler, Phys. Rev. B 75, 155435 (2007) [Selected for publication in the the May 14, 2007 issue of Virtual Journal of Nanoscale Science & Technology]
- 30. "Correlated variation of melting and Curie temperatures of nickel clusters" A. N. Andriotis,
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- 31. "Topotactic Intercalation of a Metallic Dense Host Matrix Chalcogenide with Large Electron-Phonon Coupling: Crystal Structures and Electronic Properties of $Li_xMo_2SbS_2$ ($0 \le x \le 0.7$)" A. Lappas, C. J. Nuttall, **Z. G. Fthenakis**, V. Yu. Pomajakushin, and M. A. Roberts, Chem. Mater. **19**, 69, (2007)
- 32. "Theoretical study of the effect of temperature on the magnetism of transition metal clusters" A. N. Andriotis, Z. G. Fthenakis, M. Menon, Europhys. Lett. 76, 1088, (2006)
- 33. "Applicability of the Hunjan Ramaswamy global optimization method" Z. G. Fthenakis, Phys. Rev. E 70, 066704 (2004)
- 34. "Temperature evolution of structural and magnetic properties of transition metal clusters"
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35. "A tight – binding molecular dynamics study of Ni_mSi_n binary clusters" A. N. Andriotis, M. Menon, G. Froudakis, Z. Fthenakis, and J. E. Lowther, Chem. Phys. Lett. 292, 487 (1998)

Conference Publications in Journals with Referees

1. "Study of the Si fullerene cage isomers" Z. G. Fthenakis, R. W. A. Havenith, M. Menon, and P. W. Fowler, Journal of Phys.: Conf. Series 10, 117 (2005)

Chapters in books

 "Variation of the Surface to Bulk Contribution to Cluster Properties" A. N. Andriotis, Z. G. Fthenakis and Madhu Menon, Handbook of Computational Chemistry, 2012, p. 939, Springer, Editor: T. Leszczynski

In preparation

- 1. *"Electro-magnetic induced properties of polycrystaline graphene under progressive stress: a simulation study"* (**Z. G. Fthenakis** and V. Tozzini) (to be submitted soon)
- "Electronic properties of Si₂BN nanoribbons" (M. Jaishi, B. Narayanan, Z. G. Fthenakis, A. N. Andriotis and M. Menon) (to be submitted soon)
- 3. "The importance of second neighbor interactions and other inaccuracies in molecular mechanics models for 2-fold coordinated carbon systems: The case of octagraphene" (Z. G. Fthenakis, V. Tozzini and N. N. Lathiotakis) (to be submitted soon)
- 4. "Effect of random fields in the phase transition of perovskites" (Z. G. Fthenakis and I. Ponomareva) (to be submitted soon)
- 5. "Structural and electronic properties of 3-dimensional Carbon honeycombs" (Z. G. Fthenakis) (to be submitted soon)
- 6. "Stretching graphite to diamond" (Z. G. Fthenakis and D. Tománek) (to be submitted soon)
- 7. "Electronic and mechanical properties of T8 Carbon" (Z. G. Fthenakis)
- 8. "Predicting spin polarizations of diluted magnetic ZnO" (**Z. G. Fthenakis**, A. N. Andriotis and M. Menon)
- 9. "How to make graphite from nanotubes: an intercalation pathway for graphite" (Z. G. Fthenakis and D. Tománek)
- 10. "Nanotube deformations under compression: a systematic ab-initio study" (Z. G. Fthenakis and D. Tománek)
- 11. "Energetics of Carbon fullerenes" (Z. G. Fthenakis)
- 12. "Estimation of melting temperature of small Ni clusters using classical potentials" (Z. G. Fthenakis)

Oral Presentations in Conferences

- 1. "Chemisorption of small Ni clusters on Si(110) surface" (XIIV Pan-hellenic Conference on Solid State Physics Ioannina Greece 1998)
- 2. "Adequacy of the classical potentials for the study of thermodynamic properties of transition metal clusters" (XIIX Pan-hellenic Conference on Solid State Physics Heraklion Greece 2002)

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- 3. "Study of the Si fullerene cage isomers" (Second Conference on Microelectronics Microsystems and Nanotechnology Athens Greece 2004)
- "Linear relationship between Melting and Curie temperature of Ni-clusters". Contribution of A.N. Andriotis, Z. G. Fthenakis and M. Menon at the XXIII Pan-hellenic Conference on Solid State Physics and Material Science – Athens – Greece (2007) (Proceedings, page 126)
- "Comparison of percent body fat estimations in adolescents using four different field methods". Contribution of V. Zafiropulos, Z. G. Fthenakis, D. Balaska, A. Markaki, P. Dimitropoulakis, G. A. Fragkiadakis, E. Andrioti and I. Giakoumaki at the 3rd Balkan Congress on Obesity, Thessaloniki, Greece, 17-19 Oct. 2008. (Proceedings, page 36)
- 6. *"Energy of small fullerene isomers"*. XXVI Pan-hellenic Conference on Solid State Physics and Material Science, Ioannina, Greece, (2010)
- "Computational study of the thermal conductivity of defective carbon nanostructures". Contribution of Z. G. Fthenakis and D. Tománek at the <u>APS March Meeting</u>, Boston, USA, (2012)
- 8. "A theoretical study of graphene and its planar allotropes under extreme uniaxial strain". Contribution of N. N. Lathiotakis and Z. G. Fthenakis at the <u>European</u> <u>conference/workshop on the synthesis, characterization and applications of graphene</u>, Myconos, Greece (2012)
- 9. "Can graphene allotropes surpass the high thermal conductivity of graphene?" Contribution of Z. G. Fthenakis, Z. Zhu and D. Tománek at the <u>APS March Meeting</u>, Baltimore, USA (2013)
- 10. "Deformations and nanomechanical energy storage in twisted carbon nanotube ropes". Contribution of D. Tománek, Z. G. Fthenakis, D. Teich and G. Seifert at the <u>APS March</u> <u>Meeting</u>, Baltimore, USA (2013)
- 11. "Electronic and transport properties of 2D graphene-haeckelite hybrid structures". Contributed talk of Z. Zhu, Z. G. Fthenakis and D. Tománek at CECAM workshop on "Novel 2D materials: tuning electronic properties on the atomic scale", Bremen, Germany (2013)
- 12. "Electronic and transport properties of 2D graphene-haeckelite hybrid structures". Contributed talk of Z. Zhu, Z. G. Fthenakis and D. Tománek at the International Symposium on <u>"Flatlands beyond Graphene"</u> at the Jacobs University Bremen, Germany (2013)
- 13. "Ropes of carbon nanotubes: from natural coiling to nanomechanical energy storage". Contribution of David Tománek, David Teich, Zacharias G. Fthenakis, Gotthard Seifert, and Sumio Iijima at the <u>NT13: Fourteenth International Conference on the Science and Application of Nanotubes</u> in Espoo, Finland, June 27, 2013.
- 14. "Mechanical properties of graphene, graphene nanoribbons and planar allotropes: A theoretical study". Contribution of N. N. Lathiotakis, G. Kalosakas, Z. G. Fthenakis, C. Galiotis and K. Papagelis at the <u>XXIX Panhellenic Conference on Solid-State Physics and Materials Science</u> in Athens, Greece, September 25, 2013.
- 15. "Can nanomechanical energy storage in twisting nanotube ropes surpass that of Li-ion batteries?" Contribution of Z. G. Fthenakis, D. Teich, Z. Zhu, G. Seifert and D. Tománek at the XXIX Panhellenic Conference on Solid-State Physics and Materials Science in Athens, Greece, September 25, 2013.
- 16. "Unusual conduction mechanism at graphitic carbon foam surfaces: An ab initio study". Contribution of D. Tománek, Z. Zhu, Z. G. Fthenakis and J. Guan at the <u>APS March</u> <u>Meeting</u>, Denver, Colorado, USA (2014)

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- 17. "Thermal and electrical conductivity of defective graphene: From grain boundaries to haeckelites". Contribution of Z. Zhu, Z. G. Fthenakis and D. Tománek at the <u>APS March</u> <u>Meeting</u>, Denver, Colorado, USA (2014)
- 18. "Understanding the conduction mechanism of carbon foam surfaces". Contribution of Z. G. Fthenakis, Z. Zhu, J. Guan and D. Tománek at the <u>XXX Panhellenic Conference of Solid-State Physics and Materials Science</u> in Heraklion, Greece, September 22, 2014
- 19. "<u>The effect of periodically arranged Stone-Walles defect in graphene on its mechanical properties: an ab-initio study</u>" Contribution of Z. G. Fthenakis, N. N. Lathiotakis at the <u>XXXIPanhellenic Conference o Solid-State Physics and Materials Science</u> in Thessaloniki, Greece, September 23, 2015
- 20. <u>"Ultrafast dynamics of PbZrO₃ thin films under AC electric fields</u>" Conribution of Z. G. Fthenakis and Inna Ponomareva at the <u>Foundamental Physics of Ferroelecrtics and related materials (Ferro-2019)</u> in Tampa, Florida, USA, January 27, 2019
- 21. "<u>Predicting properties of ferroelectrics with phase competitions from atomistic modeling</u>" Contribution of S. Lisenkov, M. Kingsland, D. Pappas, Z. Fthenakis and I. Ponomareva at the <u>Foundamental Physics of Ferroelecrtics and related materials (Ferro-2019)</u> in Tampa, Florida, USA, January 27, 2019
- "<u>Phase evolution in BaTi_{1-x}Zr_xO₃ from atomistic simulations</u>" Contribution of C. Mentzer, S. Lisenkov, D. Pappas, Z. Fthenakis and I. Ponomareva at the <u>Foundamental Physics of</u> <u>Ferroelecrtics and related materials (Ferro-2019)</u> in Tampa, Florida, USA, January 27, 2019
- 23. "<u>Theoretical ab-initio study of graphene vacancies and pyridinic defects for gas separation</u>" Contribution of N. N. Lathiotakis, Z. G. Fthenakis and D. Petsalakis at the Advances and applications in carbon related nanomaterials: From pure to doped structures including heteroatom layers (HeteroNanoCarb-2019), Centro de Ciencias de Benasque Pedro Pascual, Benasque, Spain, December 9, 2019
- 24. "Successes and Failures of ReaxFF potentials for 3-fold coordinated carbon systems and graphene interactions with small molecules and atoms" Contribution of Z. G. Fthenakis, I. D. Petsalakis, V. Tozzini and N. N. Lathiotakis, AutoCheMo International Reactive Force Field Workshop, Ghent, Belgium, December 8, 2021
- 25. "An algorithm for the generation, identification and enumeration of graphene pores, flakes and edges in an effective and systematic way" Zacharias G. Fthenakis, 33rd IUPAP Conference on Computational Physics (CCP2022), The University of Texas at Austin, Austin, Texas, USA, August 1 – 4, 2022
- 26. (Invited) "<u>Gas separation utilizing graphene membranes: a theoretical study</u>" Contribution of Z. G. Fthenakis, A. Fountoulakis, I. D. Petsalakis and N. N. Lathiotakis, European Assembly of Advanced Materials Congress, Stockholm, Sweden, August 28-31, 2022
- 27. "A nomenclature scheme for pores, flakes, and edges of honeycomb lattices and an algorithm for their generation and numbering", **Z.G.Fthenakis**, 37th Panhellenic Conference on Solid State Physics and Materials Science. Thessaloniki 17-20 Sept. 2023
- "In silico design of advanced graphene-based nanodevices", L. Bellucci, G. Menichetti, F. Delfino, Z. G. Fthenakis, T. T. Mamo and V. Tozzini, 2023 IEEE Natontechnology Materials and Devices Conference (NMDC) Paestrum, Italy, 2023

Other Oral Presentations

1. "Guiding nanomanufacturing research using modeling: Examples" (Center for high-rate nanomanufaturing - Northeastern University, Boston, USA, 2012)

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- 2. "Thermal conductivity of defective carbon nanostructures and Unusual electrical conduction mechanism at graphitic foam surfaces" (Invited talk at Materials Science Dept. Univ. of Crete, Greece 2013)
- "Evaluation of ReaxFF potentials for the interactions between 3-fold coordinated carbon systems and molecules" (Colloquium - Instituto Nanoscienze Consiglio Nazionale Delle Ricerche, Pisa, Italy – 2022)

Poster Presentations in Conferences

- "Study of the W_n, n<55 clusters with the Tight Binding Molecular Dynamics" Z. G. Fthenakis, A. N. Andriotis, M. Menon, N. N. Lathiotakis, XII Pan-hellenic Conference on Solid State Physics – Heraklion – Greece (1996)
- "Chemisorption of small Si clusters from the Si(110) surface" Z. G. Fthenakis, N. N. Lathiotakis, M. Menon, and A. N. Andriotis, XIII Pan-hellenic Conference on Solid State Physics – Thessaloniki – Greece (1997)
- *3.* "Study of the Si_{45} cluster" **Z. G. Fthenakis**, P. W. Fowler, and A. N. Andriotis, XIIX Panhellenic Conference on Solid State Physics Heraklion Greece (2002)
- "Study of the Si₃₈ fullerene-like cages" Z. G. Fthenakis, G. Froudakis, R. Havenith, M. Menon, P. W. Fowler, and A. N. Andriotis, XIIX Pan-hellenic Conference on Solid State Physics Heraklion Greece (2002)
- "Uncovering the FUTREX-6100XL prediction equation for the percent body fat" Z.G. Fthenakis, D. Balaska and V. Zafiropulos, 3rd Balkan Congress on Obesity, Thessaloniki, Greece, 17-19 Oct. (2008) (Proceedings, page 52)
- 6. "Clusters of transition metal atoms at non-zero temperatures" Z. G. Fthenakis, A. N. Andriotis, and M. Menon, Cluster-Surface Interactions: EuroConference on Functional Clusters (Granada June 2002)
- "Temperature evolution of structural and magnetic properties of large Ni clusters" Z. G. Fthenakis, A. N. Andriotis, and M. Menon, Cluster-Surface Interactions: EuroConference on Functional Clusters (Giens – France 2004)
- "Topotactic lithium intercalation and electronic properties in the nanostructured Mo₂SbS₂" A. Lappas, C. J. Nuttall, Z. G. Fthenakis, V. Y. Pomajakushin and M. A. Roberts, Fifth International Conference on Inorganic Materials (Ljubljana, Slovenia, 2006)
- "Correlated Variation of Melting and Curie Temperatures of Ni- clusters". A. N. Andriotis,
 Z. G. Fthenakis and M. Menon, 5th International Symposium on Theory of Atomic and Molecular Clusters (TAMC V), Richmond, VA (USA) 3-17 May, (2007) (poster no 39)
- "Linear relationship between Melting and Curie temperature of Ni-clusters" A.N. Andriotis,
 Z. G. Fthenakis and M. Menon, 6th International Conference of Fine Particle Magnetism, Rome, Italy, (2007) (poster no PB5)
- 11. "A new prediction equation for the percent body fat for adolescents, using the near infra red interactance method" Z.G. Fthenakis, I. Giakoumaki, A. Markaki and V. Zafiropulos, 17th European Congress on Obesity, Amsterdam, The Netherlands, (2009)
- 12. "Percent body fat in adolescents: Use of four field methods in a nutritional intervention" V. Zafiropulos, D. Balaska, Z. G. Fthenakis, A. Markaki, P. Dimitropoulakis, G. A. Fragkiadakis and I. Giakoumaki, 17th European Congress on Obesity, Amsterdam, The Netherlands, (2009)
- 13. "Energy of fullerenes" Z. G. Fthenakis Fullerene Silver Anniversary Symposium, Herissonisos, Crete, Greece (2010) (poster no 26)

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- 14. "Energetics of graphene clusters" Z. G. Fthenakis, 3rd international conference from nanoparticles and nanomaterials to nanodevices and nanosystems, Herissonisos, Crete, Greece (2011)
- 15. "A theoretical study of graphene and its planar allotropes under extreme uniaxial strain" N. N. Lathiotakis and Z. G. Fthenakis, International symposium and workshop on electron correlations and materials properties of compounds and alloys, Porto Heli, Greece (2012)
- 16. "The Archimedes-III nutrition-education programm 2013 2015: Assessment of growth in primary school children in Crete, Greece" V. Chatzi, A. Markaki, A. S. Kalamari, N. Thalassinos, P. Dimitropoulakis, Z. Fthenakis, N. Koufaki, I. Mavrikakis, Y. Manios, G. A. Fragkiadakis and V. Zafiropulos, DIETS-EFAD VIIIth Conference "Health 2020: Supporting Vulnerable groups", Athens (2014)
- 17. "Preliminary results of dietary intervention among primary-school choldren" V. Zafiropulos, V. Chatzi, P. Dimitropoulakis, A. Markaki, Z. G. Fthenakis, N. Thalassinos, G. A. Fragkiadakis, 22nd European Congress on Obesity (ECO2015), Prague, Czech Republic (2015)
- "Longitudinal study of intracellular water and growth in children aged 8-11 years" V. Zafiropulos, V. Chatzi, G. Giagkidis, K. Moudanos, P. Dimitropoulakis, A. Markaki, Z. G. Fthenakis, G. A. Fragkiadakis, 22nd European Congress on Obesity (ECO2015), Prague, Czech Republic (2015)
- 19. "Recording childhood obesity based on the body fat percentage before and after dietary intervention" (translated from Greek), V. Zafiropulos, A. Markaki, N. Thalassions, P. Dimitropoulakis, V. Chatzi, Z. Fthenakis, G. A. Fragkiadakis, Y. Manios and A. Kafatos, 7th Congress of the Hellenic Atherosclerosis Society, Athens (2016)
- 20. "Pseudoelectric and pseudomagnetic field in strained polycrystalline graphene: a theoretical study" **Z.G.Fthenakis** and V.Tozzini, 37th Panhellenic Conference on Solid State Physics and Materials Science. Thessaloniki 17-20 Sept. 2023

Lecture notes

Lecture notes for courses of the Department of Human Nutrition and Dietetics – Hellenic Mediterranean University - Greece

- Physics
- Physics laboratory
- Human body composition laboratory
- Introduction to error analysis (will be published as a book)

Lecture notes for courses of the Department of Civil Engineering Instructors - School of Pedagogical & Technological Education (ASPETE) – Greece

Numerical Analysis

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