Zacharias G. Fthenakis

Phone number :
website :

e-mail

1. CURRICULUM VITAE

Personal Information

Date and Place of birth :
Marital status :
Military service :
Nationality :
Languages :

Education

Ph.D. Computational Condensed Mater Physics **May 2010**
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

M.Sc Condensed Matter Physics **Sept. 1996**
University of Crete, Heraklion, Greece

B.Sc. in Physics **Nov. 1994**
University of Crete, Heraklion, Greece
grade: 7.97/10 (Upper Second-Class Honours "II.1")

Research Interests

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

Awards

Competition of the Hellenic Mathematical Society **1988**
Summer School of Advanced Physics. Univ. of Crete **1993**
IOP Trusted Reviewer **2020**

11/5/2023

Scholarships

- 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)

Employment

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* **Feb. – Jul. 2020**
- *University of West Attica, Greece* **Feb. 2020 – Sept.2021**

Research Associate **June – Aug. 2001**

- *University of Exeter, UK*

Supervisor: 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 **May 2021 - today**

Participation in scientific projects

1. EU-GROWTH AM-MARE G5RD-CT-2001-00478 (FORTH, Greece)
2. EU-TMR Network "USEFULL" (University of Exeter, UK)
3. ARCHIMEDES II (TEI of Crete, Greece)
4. NSF Cooperative Agreement no. EEC-0832785, (Michigan State University, USA)
5. THALES code MIS: 380252 (FORTH, Greece)
6. ARCHIMEDES III (MIS: 380353) (TEI of Crete, Greece)
7. DOE Grant no. DE-SC0005254 (University of South Florida, USA)
8. FLAG-ERA_"GATES" JTC-PCI2018-093137 (NHRF, Greece)
9. MONSTRE-2D PRIN2017 KFMJ8E (IN-CNR, Italy)

Professional (teaching) Experience

A. **Teaching assistant** **1992 - 1998**

Department of Physics, University of Crete, Greece

Courses:

- 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)

11/5/2023

B. <u>Instructor - Adjunct Professor - Visiting Assistant Professor</u>

1. *Hellenic Mediterranean University, Greece*
2000 – 2002, 2003 – 2011, 2013 – 2016

Department of Human Nutrition and Dietetics
<u>Courses:</u>

- 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
- Human Body Composition — spring 2015 – 2016

Department of Electrical Engineering
<u>Courses:</u>

- Electronics I — 2001 – 2002
- Electrotechincs — 2006 – 2007

Department of Agricultural Technology
<u>Courses:</u>

- Physics — fall 2014 – 2015
- Physics — fall 2015 – 2016

2. School of Pedagogical & Technological Education (ASPAITE), Greece **spring 2019-2020**

Department of Civil Engineering Instructors
<u>Courses:</u>

- Numerical Analysis — spring 2019 – 2020

3. University of West Attica, Greece **2019-2021**

Department of Surveying and Geoinformatics Engineering
<u>Courses:</u>

- Physics I — spring 2019 – 2020 & 2020 – 2021

11/5/2023

Department of Marine Engineering
Courses:
- Physics II — spring 2019 – 2020 & 2020 – 2021

Department of Wine, Vine and Beverage Sciences
Courses:
- Physics — fall 2020 – 2021

Department of Conservation of Antiquities and Works of Art
Courses:
- Physics — fall 2020 – 2021

Department of Electrical and Electronic Engineering
Courses:
- Electrical Circuits I — fall 2020 – 2021
- Electrotechnics and Electronic Technology — spring 2020 – 2021

C. Other teaching experience **2000 – 2007**
Institutes of Vocational Training, Crete, Greece
Teaching Physics and Informatics

Mentoring and supervision of students

Undergraduate thesis advisor – Hellenic Mediterranean University, Greece
1. Dimitra Mpalaska
2. Iliopoulos Sotiris
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 Pappas, Master student
3. Charles Mentzer, Undergaduate student
4. Kelli Ann Lynch, Undergraduate student

Editor

Crystals (Guest Editor for a special issue on the topic "*Density functional theory on two-dimensional materials*")

Referee in > 30 Scientific journals (impact factor in parenthesis)

- **IOP Trusted Reviewer** (awarded 2020)
- Energy & Environmental Science (25.427)
- Nano Letters (13.779)
- Nature Communications (11.878)
- Carbon (9.594)
- Nanoscale (7.760)
- Physical Review Letters (7.625)
- ACS Applied Nanomaterials (expected 7.5 – 10)
- ACS Applied Materials & Interfaces (7.145)
- 2D Materials (7.042)
- ChemComm (6.567)
- Advanced Electronic Materials (6.312)
- Advanced Materials Interfaces (4.834)

11/5/2023

- Physical Chemistry – Chemical Physics (4.449)
- Scientific Reports (3.998)
- Nanotechnology (3.953)
- Physical Review B (3.718)
- RSC Advances (3.708)
- Journal of Chemical Physics (3.488)
- Journal of Physics D: Applied Physics (3.169)
- Applied Physics Letters (3.142)
- Physica Status Solidi – Rapid Research Letters (3.032)
- Journal of Alloys and Compounds (3.014)
- The Journal of Physical Chemistry
- Physics Script (2.787)
- Journal of Physics: Condensed Matter (2.707)
- Physical Review A (2.765)
- ACS Omega (2.584)
- Journal of Applied Physics (2.370)
- Chemical Physics (2.348)
- Diamond and related materials (2.232)
- Superlattices and Microstructures (2.117)
- Computational Materials Science (2.086)
- Physica B (1.453)
- Materials Research Express (1.449)
- Key Engineering Materials (0.350)

Computing Skills

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)

1. Generation and enumeration of graphene pores with fixed number of 2-fold coordinated carbon atoms in the pore boundary (see *Carbon* **199**, 508 (2022))
2. Construction of graphene pore structures using the nomenclature scheme proposed in *Carbon* **199**, 508 (2022)
3. 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, submitted *RSC Advances - 2023*)
4. Construction of graphene flakes and (periodic) edges using the nomenclature scheme proposed in *Carbon* **199**, 508 (2022). (Generalization of the code for pores, submitted *RSC Advances – 2023*)
5. Calculation of the electronic structure of any crystal using the Harrisson's tight binding scheme
6. Molecular dynamics code using either a tight binding Hamiltonian or classical potentials
7. Calculation of (i) the rehybridized orbitals in non-planar sp^2 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

11/5/2023

8. Energy and force calculations of 10 classical potentials for transition metal systems (clusters or bulk structures) used in molecular dynamics and Monte Carlo simulations
9. Energy and force calculations for Tersoff potential used in molecular dynamics and Monte Carlo simulations. The code also calculates force contributions from each atom for thermal conductivity calculations using the non-equlibrium molecular dynamics method.
10. Phonon band structure calculation using the frozen phonon method. The code may calculate directly the forces of a classical potential if the appropriate code for the classical potential is included, or it may calculate the phonon band structure using the forces from a file. The code is appropriate both for molecules or extended systems.
11. A multiple histogram method code for calculations of thermodynamic quantities obtained using molecular dynamics or Monte Carlo simulations.
12. Improvement of the effective Hamiltonian molecular dynamics code, which is used for simulations of ferroelectric materials, to include interactions from antiferrodistortive local modes.
13. Calculation of the pseudomagnetic ans pseudoelectric field in distorted graphene structures

Schools

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)

Current *Collaborators*

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Former *Collaborators*

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11/5/2023

2. LIST OF PUBLICATIONS

Refereed articles in international journals

1. *"Graphene membranes for gas separation" (**Z. G. Fthenakis**, N. N. Lathiotakis and I. D. Petsalakis) (submitted - 2023)*
2. *"A generalized nomenclature scheme for graphene pores, flakes and edges, and an algorithm for their generation and enumeration", **Z. G. Fthenakis**, (submitted RSC Advances - 2023)*
3. "*Evaluating the performance of ReaxFF potentials for sp^2 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)
4. "*A proposed nomeclature 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)
5. *"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)
6. "*High temperature stability, metalic character and bonding of Si_2BN planar structure*" **Z. G. Fthenakis**, M. Jaishi, B. Narayanan, A. N. Andriotis and M. Menon, J. Phys. Cond. Matter **33**, 165001 (2021)
7. "*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)
8. "*Structural deformations and mechanical properties of Si_2BN 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)
9. "*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)
10. "*Intrinsic dynamics of electric-field-induced phase switching in antiferroelectric $PbZrO_3$ ultrathin films*" **Z. G. Fthenakis** and I. Ponomareva, Phys. Rev. B **98**, 054107 (2018)
11. "*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)
12. "*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)
13. "*Dynamics of antiferroelectric phase transition in $PbZrO_3$*", **Z. G. Fthenakis** and I. Ponomareva, Phys. Rev. B **96**, 184110 (2017)
14. "*Atomistic potential for graphene and other sp^2 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)
15. "*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**, 175401 (2017) *[This paper was highlighted as being particularly significant to the scientific community and is featured on JPhys+ blog.]*

11/5/2023

16. *"Are the experimentally observed 3-dimensional Carbon honeycombs, all-sp^2 structures? The dangling p-orbital instability."* **Z. G. Fthenakis,** RSC Adv. **7**, 9790 (2017)
17. *"Ab-initio investigation on the stability of H-6 Carbon",* **Z. G. Fthenakis,** RSC Adv. **6**, 78187 (2016)
18. *"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)*
19. *"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)*
20. *"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)
21. *"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)
22. *"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)*
23. *"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)*
24. *"Energetics of graphene flakes"* **Z. G. Fthenakis,** Mol. Phys. **111**, 3289 (2013)
25. *"Nanomechanical energy storage in twisted nanotube ropes" D. Teich,* ***Z. G. Fthenakis****, G. Seifert, and D. Tománek, Phys. Rev. Lett.* ***109****, 255501 (2012)*
26. *"Computational study of the thermal conductivity in defective carbon nanostructures"* **Z. G. Fthenakis,** and D. Tománek, Phys. Rev. B **86**, 125418 (2012)
27. *"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)
28. *"Structural and electronic properties of the fullerene isomers of Si_{38}: 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*]*
29. *"Correlated variation of melting and Curie temperatures of nickel clusters"* A. N. Andriotis, **Z. G. Fthenakis,** and M. Menon, Phys. Rev. B **75**, 073413 (2007) *[Selected for publication in the the March 12, 2007 issue of* Virtual Journal of Nanoscale Science & Technology*]*
30. *"Topotactic Intercalation of a Metallic Dense Host Matrix Chalcogenide with Large Electron-Phonon Coupling: Crystal Structures and Electronic Properties of $Li_xMo_2SbS_2$ ($0 \leq x \leq 0.7$)"* A. Lappas, C. J. Nuttall, **Z. G. Fthenakis** , V. Yu. Pomajakushin, and M. A. Roberts, Chem. Mater. **19** , 69, (2007)
31. *"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)
32. *"Applicability of the Hunjan - Ramaswamy global optimization method"* **Z. G. Fthenakis,** Phys. Rev. E **70**, 066704 (2004)
33. *"Temperature evolution of structural and magnetic properties of transition metal clusters"* **Z. Fthenakis**, A. N. Andriotis, and M. Menon, J. Chem. Phys. **119**, 10911 (2003)

11/5/2023

34. *"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

1. *"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)
2. "*Electronic properties of Si_2BN nanoribbons*" (M. Jaishi, B. Narayanan, **Z. G. Fthenakis**, A. N. Andriotis and M. Menon) (to be submitted soon)
3. "Effect *of random fields in the phase transition of perovskites*" (**Z. G. Fthenakis** and I. Ponomareva) (to be submitted soon)
4. "*Structural and electronic properties of 3-dimensional Carbon honeycombs*" (**Z. G. Fthenakis**) (to be submitted soon)
5. *"Stretching graphite to diamond"* (**Z. G. Fthenakis** and D. Tománek) (to be submitted soon)
6. "*How many Si_2BN planar structures are they?*" (**Z. G. Fthenakis**, A. N. Andriotis and M. Menon)
7. "*Unisotropic behaviour of 2D structures with Octagraphene topology under uniaxial strain*" (**Z. G. Fthenakis** and N. N. Lathiotakis) (to be submitted soon)
8. *"Electronic and mechanical properties of T8 Carbon" (***Z. G. Fthenakis***)*
9. *"Predicting spin polarizations of diluted magnetic ZnO" (***Z. G. Fthenakis**, A. N. Andriotis and M. Menon*)*
10. *"How to make graphite from nanotubes: an intercalation pathway for graphite"* (**Z. G. Fthenakis** and D. Tománek)
11. *"Nanotube deformations under compression: a systematic ab-initio study"* (**Z. G. Fthenakis** and D. Tománek)
12. *"Energetics of Carbon fullerenes"* (**Z. G. Fthenakis**)
13. *"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)

11/5/2023

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)
3. *"Study of the Si fullerene cage isomers"* (Second Conference on Microelectronics Microsystems and Nanotechnology – Athens – Greece 2004)
4. *"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)
5. *"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)
7. *"Computational study of the thermal conductivity of defective carbon nanostructures"*. Contribution of Z. G. Fthenakis and D. Tománek at the APS March Meeting, 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 European conference/workshop on the synthesis, characterization and applications of graphene, 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 APS March Meeting, 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 APS March Meeting, 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 "Flatlands beyond Graphene" 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 NT13: Fourteenth International Conference on the Science and Application of Nanotubes 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 XXIX Panhellenic Conference on Solid-State Physics and Materials Science 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.

11/5/2023

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 APS March Meeting, Denver, Colorado, USA (2014)
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 APS March Meeting, 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 XXX Panhellenic Conference of Solid-State Physics and Materials Science in Heraklion, Greece, September 22, 2014
19. "*The effect of periodically arranged Stone-Walles defect in graphene on its mechanical properties: an ab-initio study*" Contribution of Z. G. Fthenakis, N. N. Lathiotakis at the XXXIPanhellenic Conference o Solid-State Physics and Materials Science in Thessaloniki, Greece, September 23, 2015
20. "*Ultrafast dynamics of $PbZrO_3$ thin films under AC electric fields*" Conribution of Z. G. Fthenakis and Inna Ponomareva at the Foundamental Physics of Ferroelecrtics and related materials (Ferro-2019) in Tampa, Florida, USA, January 27, 2019
21. "*Predicting properties of ferroelectrics with phase competitions from atomistic modeling*" Contribution of S. Lisenkov, M. Kingsland, D. Pappas, Z. Fthenakis and I. Ponomareva at the Foundamental Physics of Ferroelecrtics and related materials (Ferro-2019) in Tampa, Florida, USA, January 27, 2019
22. "*Phase evolution in $BaTi_{1-x}Zr_xO_3$ from atomistic simulations*" Contribution of C. Mentzer, S. Lisenkov, D. Pappas, Z. Fthenakis and I. Ponomareva at the Foundamental Physics of Ferroelecrtics and related materials (Ferro-2019) in Tampa, Florida, USA, January 27, 2019
23. "*Theoretical ab-initio study of graphene vacancies and pyridinic defects for gas separation*" 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)** *"Gas separation utilizing graphene membranes: a theoretical study"* 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

Other Oral Presentations

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

11/5/2023

3. "*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

1. *"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)
2. *"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 Pan-hellenic Conference on Solid State Physics – Heraklion – Greece (2002)
4. *"Study of the Si_{38} 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)
5. *"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)
7. *"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)
8. *"Topotactic lithium intercalation and electronic properties in the nanostructured Mo_2SbS_2"* A. Lappas, C. J. Nuttall, **Z. G. Fthenakis** , V. Y. Pomajakushin and M. A. Roberts, Fifth International Conference on Inorganic Materials (Ljubljana, Slovenia, 2006)
9. *"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)
10. *"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)
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)
18. "Long*itudinal 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)

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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