
Zacharias G. Fthenakis

LIST OF PUBLICATIONS

Refereed articles in international journals

1. “Understanding the metallic character and bonding of Si_2BN planar structure” **Z. G. Fthenakis**, A. N. Andriotis and M. Menon (submitted to J. Phys. Cond. Matter (2020))
2. “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)
3. “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)
4. “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)
5. “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)
6. “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)
7. “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)
8. “Dynamics of antiferroelectric phase transition in $PbZrO_3$ ”, **Z. G. Fthenakis** and I. Ponomareva, Phys. Rev. B **96**, 184110 (2017)
9. “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)
10. “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. “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)
12. “Ab-initio investigation on the stability of H-6 Carbon”, **Z. G. Fthenakis**, RSC Adv. **6**, 78187 (2016)
13. “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)
14. “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)

15. "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)
16. "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)
17. "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)
18. "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)
19. "Energetics of graphene flakes" **Z. G. Fthenakis**, Mol. Phys. **111**, 3289 (2013)
20. "Nanomechanical energy storage in twisted nanotube ropes" D. Teich, **Z. G. Fthenakis**, G. Seifert, and D. Tománek, Phys. Rev. Lett. **109**, 255501 (2012)
21. "Computational study of the thermal conductivity in defective carbon nanostructures" **Z. G. Fthenakis**, and D. Tománek, Phys. Rev. B **86**, 125418 (2012)
22. "Uncovering the FURTEX-6100XL prediction equation for the percent body fat" **Z. G. Fthenakis**, D. Balaska, and V. Zafirooulos, J. Med. Eng. Technol. **36**, 351 (2012)
23. "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](#)*]
24. "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](#)*]
25. "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)
26. "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)
27. "Applicability of the Hunjan - Ramaswamy global optimization method" **Z. G. Fthenakis**, Phys. Rev. E **70**, 066704 (2004)
28. "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)
29. "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. “Gas separation utilizing graphene membranes: a theoretical study” **Z. G. Fthenakis**, A. Fountoulakis, I. D. Petsalakis and N. N. Lathiotakis, (submitted for publication in Adv. Mater. Lett. - 2020)
2. “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