Pantelis C. Kelires
Professor of Physics & Materials Science
PhD, State University of New York, USA (1987)
BSc: University of Athens, Greece (1981)
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POSITIONS

Cyprus University of Technology - Department of Mechanical & Materials Science Engineering
Professor, 2007 – present
Vice-Rector for Academic Affairs, 2020 – 2023
Director of the Research Unit "Nanostructured Materials Systems", 2010 – present
Department Coordinator, 2007 – 2010
Chairman of the University Studies Committee, 2008 – 2011
Physics Department – University of Crete
Head of the Simulational Physics / Materials Science Theory Group
Professor, 2003 – 2009
Associate Professor, 1994 – 2003
Assistant Professor, 1989 – 1994
Foundation for Research and Technology-Hellas, Institute of Electronic Structure and Laser
Affiliated faculty member, 1989 – 2004
IBM Research Division, T.J. Watson Research Center, Yorktown Heights, USA
Postdoctoral researcher, 1987 – 1989

RESEARCH INTERESTS

Computational Materials Science – Condensed Matter Physics; Structural and optoelectronic properties of crystalline and amorphous materials; Nanomaterials (quantum dots, nanostructured and nanocomposite materials, nanocrystals); Optoelectronic properties of amorphous and nanostructured carbon; Phase transitions, order-disorder phenomena (phase diagrams of crystalline alloys); Stability of superlattices and heterostructures; Chemical ordering in alloyed systems; Expertise in Monte Carlo simulations, development of novel algorithms (introduction of the semi-grand canonical ensemble to equilibrate semiconductor alloys); Tight-binding molecular dynamics and *ab initio* methods; Statistical approach to problems of disorder; Atomic scale properties (local stresses, introduction of atomic bulk modulus).

PUBLICATIONS

Author of more than 100 articles in international peer-reviewed journals, attracting about 3000 citations, with an H-index of 32 (Scopus).

Selected publications:

1. "Glassy Quasithermal Distribution of Local Geometries and Defects in Quenched Amorphous Silicon", P. C. Kelires and J. Tersoff, Phys. Rev. Lett. 61, 562 (1988).

2. "Equilibrium Alloy Properties by Direct Simulation", P. C. Kelires and J. Tersoff, Phys. Rev. Lett. 63, 1164 (1989).

3. "Structure and Chemical Ordering in Amorphous Silicon Carbide Alloys", P. C. Kelires, Europhysics Letters 14, 43 (1991).

4. "Energetics and Stability of Diamondlike Amorphous Carbon", P. C. Kelires, Phys. Rev. Lett. 68, 1854 (1992).

5. "Structural Properties and Energetics of Amorphous Forms of Carbon", P. C. Kelires, Phys. Rev. B 47, 1829 (1993).

6. "Elastic Properties of Amorphous Carbon Networks", P. C. Kelires, Phys. Rev. Lett. 73, 2460 (1994).

7. "Monte Carlo Studies of Ternary Semiconductor Alloys", P. C. Kelires, Phys. Rev. Lett. 75, 1114 (1995).

8. "Energetics and Equilibrium Properties of Thin Pseudomorphic SiC Layers in Si", P. C. Kelires and E. Kaxiras, Phys. Rev. Lett. 78, 3479 (1997).

9. "Dimer Pairing on the C-alloyed Si(001) Surface", O. Leifeld, D. Gruetzmacher, B Mueller, K. Kern, E. Kaxiras, and P. C. Kelires, Phys. Rev. Lett. 82, 972 (1999).

10. "Intrinsic Stress and Local Rigidity in Tetrahedral Amorphous Carbon", Phys. Rev. B 62, 15686 (2000).

11. "Thermodynamics of C Incorporation on Si(100) from Ab Initio Calculations", I. N. Remediakis, E. Kaxiras, and P. C. Kelires, Phys. Rev. Lett. 86, 4556 (2001).

12. "Monte Carlo Studies of Stress Fields and Intermixing in Ge Quantum Dots", P. Sonnet and P. C. Kelires, Phys. Rev. B 66, 205307 (2002).

13. "Physical Origin of Trench Formation in Ge/Si(100) Islands", P. Sonnet and P. C. Kelires, Appl. Phys. Lett. 85, 203 (2004).

14. "Structure and Energetics of Si Nanocrystals Embedded in a-SiO2", G. Hadjisavvas, and P. C. Kelires, Phys. Rev. Lett. 93, 226104 (2004).

15. "Insights into the Fracture Mechanisms and Strength of Amorphous and Nanocomposite Carbon", M. G. Fyta, I. N. Remediakis, P. C. Kelires, and D. A. Papaconstantopoulos, Phys. Rev. Lett. 96, 185503 (2006).

16. "Simulations of Composite Carbon Films with Nanotube Inclusions", M. G. Fyta and P. C. Kelires, Appl. Phys. Lett. 86, 191916 (2005).

17. "Probing the Structure and Energetics of Dislocation Cores in SiGe Alloys through Monte Carlo Simulations", I. N. Remediakis, D. E. Jesson, and P. C. Kelires, Phys. Rev. Lett. 97, 255502 (2006).

18. "Self-assembly and Ordering Mechanisms of Ge Islands on Prepatterned Si(001)", A. Pascale, I. Berbezier, A. Ronda, and P. C. Kelires, Physical Review B 77, 075311 (2008).

19. "Softening of Ultra-Nanocrystalline Diamond at Low Grain Sizes", I. N. Remediakis, G. Kopidakis, and P. C. Kelires, Acta Materialia 56, 5340 (2008).

20. "Suppression of Intermixing in Strain-Relaxed Epitaxial Layers", T. Leontiou, J. Tersoff, and P. C. Kelires, Phys. Rev. Lett. 105, 236104 (2010).

21. "Ordering Mechanisms in Epitaxial SiGe Nanoislands", G. Vantarakis, I. N. Remediakis, and P. C. Kelires, Phys. Rev. Lett. 108, 176102 (2012).

22. "Optical and Elastic Properties of Diamond-like Carbon with Metallic Inclusions: A Theoretical Study", G. Tritsaris, C. Mathioudakis, P. C. Kelires, and E. Kaxiras, J. Appl. Phys. 112, 103503 (2012).

23. "Atomistic Simulations of Low-Density Nanoporous Materials: Carbon Nanofoams", C. Mathioudakis and P. C. Kelires , Physical Review B 87, 195408 (2013).

24. "Stress State of Embedded Si Nanocrystals", K. Kleovoulou and P. C. Kelires, Physical Review B 88, 085424 (2013).

25. "Composition and Stress of SiGe Nanostructures on Curved Substrates", T. Leontiou and P. C. Kelires, Physical Review B 93, 125307 (2016).

26. "Modeling of Three-Dimensional Nanographene", C. Mathioudakis and P. C. Kelires , Nanoscale Research Letters 11, 151 (2016).

27. **"**Temperature dependence of the optical properties of silicon nanocrystals", M. Zacharias and P. C. Kelires, Physical Review B 101, 245122 (2020).

28. "Quantum Confinement of Electron−Phonon Coupling in Graphene Quantum Dots", M. Zacharias and P. C. Kelires, J. Phys. Chem. Lett. 12, 9940 (2021).

29. "Efficient First-Principles Methodology for the Calculation of the All-Phonon Inelastic Scattering in Solids", M. Zacharias *et. al.*, Phys. Rev. Lett. 127, 207401 (2021).

PHD STUDENTS AND POSTDOCTORAL RESEARCHERS

PhD students: I. Remediakis (PhD 2002), now Associate Professor, University of Crete – C. Tzoumanekas (PhD 2003), now researcher at NTUA – M. Fyta (PhD 2005), now Group Leader at the Institute for Computational Physics, University of Stuttgart – G. Hadjisavvas (PhD 2005), now in Secondary Education – C. Mathioudakis (PhD 2007), now in Secondary Education – K. Kleovoulou (PhD 2014), now at the administration of Cyprus Institute.

Postdoctors: G. Kopidakis (1999-2001), now Associate Professor at the University of Crete – Ph. Sonnet (2000-01), now researcher at University Haute Alsace & CNRS, Mulhouse, France – C. Guedj (2000), now at LETI, Grenoble, France – A. Pascale (2003-04), now at CEA, Grenoble, France – I. Remediakis (2004-2007) – Th. Leontiou (2007-2010), now Associate Professor at Frederick University (Nicosia, Cyprus) – M. Zacharias (2019 – 2022).

FUNDING (INDICATIVE)

ESPRIT Basic Research EU Program, Project 7128: "Ultrathin Si/Ge Microstructures", (167000 ECU, 9/1992 – 9/1995).

Human Capital and Mobility EEC Program, Project 0355: "Heterostructures on Si for Integrated Optoelectronics", (35000 ECU, 11/1993 – 10/1996).

GSRT, ΕΠΕΤ II, Greece: "Calculations of Properties of New Crystalline and Amorphous Materials", (31,117,160 GRD, 1/1999 – 12/2001).

EU Research Training Network, Project RTN1-1999-00368: "SiGeC Nanostructures: a New Path to Si-based Optoelectronics", (192000 Euro, 3/2000 – 3/2004).

ΥΠΕΠΘ, Programme "ΗΡΑΚΛΕΙΤΟΣ", Greece: "Theoretical Investigation of Nanostructured Semiconductors by Monte Carlo and *ab initio* Methods", (32000 Euro, 5/2003 – 5/2006).

ΥΠΕΠΘ, Programme "ΠΥΘΑΓΟΡΑΣ", Greece: "Theoretical/Computational Study of Nanostructured Carbon Phases, a Multiscale Approach", (75000 Euro, 3/2004 – 12/2007.

Research Promotion Foundation (RPF), Programme "New Infrastructure", Cyprus: "Theoretical/Simulational Studies of Novel Carbon Nanostructures", (115000 Euro, 1/2007 – 7/2010).

RPF, Programme "ΔΙΔΑΚΤΩΡ", Cyprus: "Theory and Simulations of Si and Ge Nanocrystals in a Dielectric Amorphous Matrix", (135000 Euro, 12/2008 – 12/2011).

RPF, Programme "New Infrastructure-Strategic Infrastructure Programs", Cyprus: "Research Unit for Nanostructured Materials Systems", (2,000,000 Euro, 11/2010 – 06/2015).

CONFERENCE ORGANIZATIONS

More than 20 international and local meetings – Indicative:

"International Symposium on Si Heterostructures: from Physics to Devices", (Crete, September 1995): Co-organizer with S. Lagomarsino.

"Rigidity and strain fields in crystalline and amorphous semiconductors", CECAM workshop, (Lyon, France, June 2001): Co-organizer with M. F. Thorpe.

''Sixth Specialists Meeting on Amorphous Carbon'', SMAC 2006 (Crete, September 2006): Chairman of the Organizing Committee.

NATO Advanced Research Workshop on "Quantum Dots: Fundamentals, Applications, and Frontiers", (Crete, June 2003): Co-organizer with D. Vvedensky.

"XXVII Panhellenic Conference on Solid State Physics and Materials Science", Limassol, Cyprus, September 18-21, 2011: Chairman of the organizing committee.

E-MRS Spring Meeting 2016, Symposium EE "Carbon- or Nitrogen Containing Nanostructured Thin Films", (Lille, France): Co-organizer.

INVITED TALKS (INDICATIVE)

''Native Defects and Glassy Properties of Amorphous Silicon'', 1989 March meeting of the American Physical Society, St. Louis (USA).

''Segregation and Ordering at the SiGe(100) Surface'', 20th International Conference on the Physics of Semiconductors, Thessaloniki (Greece), August 1990.

''Review of Simulations of Amorphous Carbon Thin Films'', First Specialist's Meeting on Amorphous Carbon, Cambridge (UK), July 1997.

''Monte Carlo Simulations of Highly Strained Semiconductor Alloys'', MRS Fall Meeting, Boston (USA), November 1998.

"Structure, Stability, and Stress Properties of Amorphous and Nanostructured Carbon Films", Symposium "Synthesis, Characterization and Advanced Applications of Amorphous Carbon Films", E-MRS 2004 Spring Meeting, May 24-28, 2004, Strasbourg (France).

''Monte Carlo Simulations of Si Nanocrystals in Amorphous Silicon Dioxide'', E-MRS Spring Meeting, Strasbourg (France), May 2004.

''Simulations of Stress and Composition in Ge/Si Quantum Dots'', March Meeting of the American Physical Society, Los Angeles (USA), 2005.

''Interface Structure and Electronic Properties of Si Nanocrystals in Amorphous Silicon Dioxide'', E-MRS Spring Meeting, Strasbourg (France), May 2006.

"Simulations of Nanocomposite Carbon Films", E-MRS Fall Meeting, Warsaw (Poland), September 2006.

"Modeling of Ultra-Nanocrystalline Diamond", 4th International Conference on "Nanosciences & Nanotechnologies - NN07", Thessaloniki (Greece), July 16-18, 2007.

"Theory of Defects and Optical Properties in Si Nanocrystals Embedded in a-SiO_2", Villa Conference on Interactions Among Nanostructures 2010, Santorini (Greece), June 21-25, 2010.

"Modeling Nanostructured Materials Systems", plenary talk at the XXVI Panhellenic Conference on ``Solid State Physics and Materials Science", Ioannina (Greece), September 26-29, 2010.

"Suppression of Intermixing in Strain-Relaxed Epitaxial Layers", International Conference on Metallurgical Coatings and Thin Films, San Diego, California (USA), May 2-6, 2011.

"Atomistic Simulations of Nanostructured and Nanocomposite Carbon Films", E-MRS Spring Meeting 2012, Symposium U ``Carbon- or Nitrogen Containing Nanostructured Thin Films", Strasbourg (France).

"Stress and Composition of SiGe Nanostructures on Curved Substrates", 6th International Conference on **NANO**structures and nanomaterials **SE**lf-**A**ssembly (NANOSEA), July 3-8, 2016, Sicily (Italy).

DISTINCTIONS

Listed in the top 1% of researchers worldwide across all scientific disciplines. (*https://journals.plos.org/plosbiology/article?id=10.1371/journal.pbio.3000918*).

Outstanding Referee of the American Physical Society (2016).