XIHONG PENG

Assistant Professor,
Dept. of Applied Sciences and Mathematics, College of Technology and Innovation,
Arizona State University, Wanner 340N, 6073 S. Backus Mall, Mesa, AZ 85212
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EDUCATION

Ph. D. in Physics Aug. 2007
Rensselaer Polytechnic Institute, Troy, NY, USA
Thesis: *First principles study of size and strain effects on the electronic properties in Si and SiC nanostructures*
Advisor: Prof. Saroj K. Nayak; **Co- Advisor:** Prof. Sanat K. Kumar

B. S. in Physics Jul. 2000
Beijing Normal University, Beijing, P. R. China

PROFESSIONAL APPOINTMENTS

Assistant Professor, Arizona State University**,** Dept. of Applied Sciences and Mathematics, 2008-present
Postdoctoral Research Associate, Rensselaer Polytechnic Institute, Dept. of Physics, 2007-2008
Visiting Assistant Professor, Skidmore College, Dept. of Physics, 2007-2008

RESEARCH EXPERIENCE

Arizona State University, Dept. of Applied Sciences and Mathematics, Mesa, AZ, USA

Assistant Professor 2008-present

- NANOCAPACITORS: Explore the origin of the dielectric dead layer effect in nanoscale capacitors and simulate the performance the permittivity profile for capacitors made from perovskite ferroelectric materials
- HYDROGEN STORAGE: Investigate hydrogenation/dehydrogenation in novel Pd-coated Mg nanoblades
- GRAPHENE: Study the electronic and transportation properties of graphene ribbon with edge functionalization, doping and defects.
- GROUP III-V SEMICONDUCTOR NANOSTRUCTURES: Study the structural and electronic properties in group III nitride nanostructures, such as quantum dots, nanowires and thin films.
- GERMANIUM/SILICON HETERO-NANOSTRUCTURES**:** Investigate the mechanical and electronic properties of core-shell structured germanium/silicon nanowires.

Rensselaer Polytechnic Institute, Dept. of Physics, Troy, NY, USA

Postdoctoral Research Associate 2007-2008

- FLUOROPHORES**:** Explored quantum confined Stark effect in organic fluorophores, such as tyrosine, tryptophan, coumarin 314, and rhodamine 123. Explained the red/blue shifts in emission spectra of organic fluorophores by the proposed concept of "local dipole moment" of molecular orbitals.
- INFRA-RED AND TERAHERTZ SPECTRA: Studies the infra-red and terahertz spectra of organic and inorganic chemicals at low temperature, such as pesticides (acephate and dimethoate)

Graduate Research Assistant 2002-2007

- SILICON NANOSTRUCTURES**:** Studied size and strain effects on the photoluminescence of Si quantum dots. Explored the electronic properties, such as band structures and carrier effective masses, in Si quantum wires. This work enables us to potentially control the wavelengths of light devices and electron and hole mobilities through size and strain variation.
- SILICON CARBIDE QUANTUM DOTS**:** Investigated the electronic, optical, and structural properties of SiC nanoclusters with varying polytype morphology (2H, 3C, and 4H) and size (0.5 ~ 2.0 nm).
- CARBON NANOTUBES**:** Calculated the electronic properties, such as band structures, density of states, effective masses of charge carrier, in carbon nanotubes.

- POLYMER-METAL INTERACTIONS**:** Studied the interactions between methyl acetate (model for PMMA) and aluminum surface as well as Al nanoclusters.
- MAGNETIC COBALT DOTS**:** Studied the surfactant mediated synthesis and supramolecular assembly of Co quantum dots through deriving interaction potentials between pairs of interacting micelles.

General Electric, Global Research Center, Niskayuna, NY, USA

Research Intern May-Aug. 2004

Research Consultant May-Dec. 2005

- NOVEL SCALING LAWS FOR BAND GAPS IN QUANTUM DOTS**:** Proposed new scaling laws that govern coupled mechanical deformation and optoelectronic properties (band gap) in quantum dots. Performed theoretic calculations, which indicate that novel size effects on band gap become operative in the 1 ~ 5 nm size range.
- SIZE DEPENDENCE IN ELASTIC STATES**:** Studied the size dependence in elastic states of nano-inclusions and inhomogeneity including surface and interface effects. Proposed the concept "surface elasticity" and evaluated it via molecular dynamics and density functional theory on Al (100) slab models.
- SILICON CARBIDE POLYTYPE TRANSFORMATION**:** Studied SiC polytype transformation, from 4H to 3C, based on the dislocation mechanism. Predicted the barrier of the phase transition. Studied the strain effect on the barrier height and found that tensile strain facilitates the phase transition.

PUBLICATIONS IN REFEREED JOURNALS

1. **X. -H. Peng,** P. Logan, "Electronic properties of strained Si/Ge core-shell nanowires" Appl. Phys. Lett **96**, 143119 (2010).
2. P. Logan, **X. -H. Peng,** "Strain Modulated Electronic Properties of Ge Nanowires – A First Principles Study", Phys. Rev. B **80**, 115322 (2009).
3. **X. -H. Peng,** A. Alizadeh, S. K. Kumar, and S. K. Nayak, "Ab-initio study of size and strain effects on the electronic properties of Si nanowires", Int. J. of Applied Mechanics **1**, 483 (2009).
4. Y. Zhang, **X. -H. Peng,** Y. Chen, A. Curino, W. Andreoni, X. Zhang, and S. K. Nayak, "A first principle study of Terahertz (THz) Spectra of Acephate", Chem. Phys. Letts. **452**, 59 (2008).
5. S. Sreekala, **X. -H. Peng,** P. M. Ajayan, and S. K. Nayak, "Effect of strain on band gap and effective mass in zigzag single-wall carbon nanotubes", Phys. Rev. B **77**, 155434 (2008).
6. **X. -H. Peng,** S. K. Nayak, A. Alizadeh, K. K. Varanasi, N. Bhate, L. B. Rowland, and S. K. Kumar, "First principles study of the effects of polytype and size on energy gaps in SiC nanoclusters", J. Appl. Phys. **102**, 024304 (2007) .
7. **X. -H. Peng,** A. Alizadeh, N. Bhate, S. K. Kumar, and S. K. Nayak, "First principles investigation of strain effects on the energy gaps in Si nanoclusters", J. Phys.: Condens. Matter **19**, 266212 (2007).
8. **X. -H. Peng,** S. Ganti, A. Alizadeh, P. Sharma, S. K. Kumar, and S. K. Nayak, "Strain engineered photoluminescence of silicon nanoclusters", Phys. Rev. B **74**, 035339 (2006).
9. K. Iyakutti, A. Bodapati, **X. -H. Peng,** P. Keblinski, S. K. Nayak, "Electronic band structure, electron-phonon interaction and superconductivity of (5, 5), (10, 10) and (5, 0) carbon nanotubes", Phys. Rev. B **73**, 035413 (2006).
10. **X. -H. Peng,** S. Ganti, P. Sharma, A. Alizadeh, S. K. Nayak, S. K. Kumar, "Novel scaling laws for band gaps of quantum dots", J. Comput. Theor. Nanosci. **2**, 469 (2005).
11. N. P. Adhikari, **X. -H. Peng,** A. Alizadeh, S. Ganti, S. K. Nayak, and S. K. Kumar, "Multiscale modeling of the surfactant mediated synthesis and supramolecular assembly of cobalt nanodots", Phys. Rev. Lett. **93**, 188301 (2004).
12. M. Zhan, Z. -G. Zheng, G. Hu, **X. -H. Peng,** "Nonlocal chaotic phase synchronization", Phys. Rev. E **62**, 3552 part A (2000).

BOOK CHAPTERS

- N. Adhikari, **X. -H. Peng,** A. Alizadeh, S. Nayak, and S. K. Kumar, "Multiscale Modeling of the Synthesis of Quantum Nanodots and their Arrays", Chapter 4, *Nanomaterials: Design and Simulation*, P. B. Balbuena & J. M. Seminario (Editors), 2007 Elsevier.

CONFERENCES TALKS AND PRESENTATIONS

1. **X. -H. Peng,** F. Tang, P. Logan, "Electronic properties of strained Si [111] nanowires", *American Physical Society, 2010 March meeting*, Portland, OR (poster presentation, 2010).
2. **X. -H. Peng,** F. Tang, P. Logan, "First Principles Study of Size and Strain Effects on the Structural and Electronic Properties in SI/Ge Core-Shell nanowires", *American Physical Society, 2009 4-Corners-Section meeting*, Golden, CO (poster presentation, 2009).
3. S. Velasquez, P. Logan, **X. -H. Peng,** "Strain and edge passivation induced band gap modulation and effective mass tuning in Armchair Graphene Nanoribbons", *American Physical Society, 2009 4-Corners-Section meeting*, Golden, CO (poster presentation, 2009).
4. P. Logan, **X. -H. Peng,** "The effects of strain and quantum confinement on the electronic properties of germanium nanowires", *American Physical Society, 2009 March meeting*, Pittsburgh, PA (oral presentation, 2009).
5. **X. -H. Peng,** J. Anderson, G. Tepper, S. Bandyopadhyay, S. Nayak, "Quantum confined Stark effect in organic fluorophores", *American Physical Society, 2008 March meeting*, New Orleans, LA (oral presentation, 2008).
6. **X. -H. Peng,** S. K. Kumar, S. K. Nayak, "First principles study of strain effects on the electronic properties in silicon nanowires", *American Physical Society, 2007 March meeting*, Denver, CO (oral presentation, 2007).
7. Y. Zhang, **X. -H. Peng,** Y. Chen, S. K. Nayak, X. -C. Zhang, "First principles simulations of THz spectra of acephate: insight into the phonon signatures", *American Physical Society, 2007 March meeting*, Denver, CO (oral presentation, 2007).
8. **X. -H. Peng,** A. Alizadeh, N. Bhate, L. B. Rowland, S. K. Nayak, S. K. Kumar, "The effect of polytype on energy gap in SiC nano-clusters", *American Physical Society, 2006 March meeting*, Baltimore, MD (oral presentation, 2006).
9. **X. -H. Peng,** A. Alizadeh, N. Bhate, S. Ganti, P. Sharma, S. Nayak, S. Kumar, "Density functional study of strain effects on the energy gap in silicon nanoclusters", *American Physical Society, 2006 March meeting*, Baltimore, MD (poster presentation, 2006).
10. N. Adhikari, **X. -H. Peng,** S. K. Nayak, S. K. Kumar, "Modeling the surfactant mediated synthesis of quantum nanodots and their arrays", *American Physical Society, 2004 March meeting*, Montreal, Quebec, Canada (oral presentation, 2004).
11. S. K. Kumar, N. Adhikari, **X. -H. Peng,** S. K. Nayak, "Multiscale modeling of the surfactant mediated synthesis and supramolecular assembly of cobalt nanodots", *American Institute of Chemical Engineers, 2004 November meeting*, Austin, TX (oral presentation, 2004).

UNIVERSITY TALKS

1. University of Houston, Houston, Department of Mechanical Engineering, "Predictive modeling for nanoscale materials using first principles calculation: -- *Photoluminescence of quantum dots and Stark effect in fluorescent molecules*", May 21st, 2009
2. Arizona State University, Tempe, Department of Physics, "Predictive modeling for nanoscale materials using first principles calculation", November 10th, 2008
3. University of Massachusetts, Dartmouth, Department of Physics, "Tunable luminescence from silicon quantum dots", March 27th, 2008
4. University of Wisconsin-Eau Claire, Department of Physics, "Tunable luminescence from silicon quantum dots", March 11th, 2008
5. Westminster College, Department of Physics, "Tunable luminescence from silicon quantum dots", February 6th, 2008
6. Skidmore College, Department of Physics, "Tunable luminescence from silicon quantum dots", April 5th, 2007
7. Rensselaer Polytechnic Institute, Department of Physics, "Silicon quantum dots", July 19th, 2006

TEACHING EXPERIENCE

- Teaching Professor for "*PHY112"* in Fall 2008, Spring and Fall 2009, Spring and Fall 2010 at Arizona State University
- Teaching Professor for course "*PHY111*" in Fall2008, Fall 2009 at Arizona State University
- Teaching Professor for courses "*General Physics II with Lab "* and "*Condensed Matter Physics "* in Spring 2008 at Skidmore College
- Teaching Professor for courses "*General Physics I with Lab "* and "*Origins of Classical Physics with Lab*" in Fall 2007 at Skidmore College

- Teaching Assistant for undergraduate STUDIO "*Physics II*" in Fall 2002 and Spring 2003 at Rensselaer Polytechnic Institute
- Teaching Assistant for graduate "*Advanced Mechanics*" in Fall 2003 at Rensselaer Polytechnic Institute
- Intern Instructor for "*Newtonian Mechanics*" in Fall 1999 at Beijing Jiaotong High School, Beijing, P. R. China

STUDENTS SUPERVISED

- Paul Logan (graduate), Spring 2009 - present
- Selina Velasquez (undergraduate), Spring, summer and fall 2009 and spring 2010
- Alan Bradford (undergraduate), Spring 2009
- Joshua Hoyt (undergraduate), Spring 2010

PROFESSIONAL AFFILIATIONS

- Member of Sigma Pi Sigma Honor Society
- Member of the American Physical Society

AWARDS

- Outstanding fellowship for academy performance 1997-2000
- Excellent intern as a high-school instructor 1999
- Yi-Zhou scholarship 1996-1997

ACADEMIC AND COMMUNITY SERVICES

Referee for the journals of Nanotechnology, Journal of Physics: Condensed Matter, New Journal of Physics, Journal of Physics: Condensed Matters, Applied Physics Letters.