

Xihong Peng, Associate Professor

Science and Mathematics Faculty, College of Integrative Sciences and Arts

Arizona State University at the Polytechnic Campus, Mesa, AZ 85212

Phone: (480) 727-5013; E-mail: xihong.peng@asu.edu;

Homepage: <http://peng.faculty.asu.edu/>Google Scholar Citations: <https://scholar.google.com/citations?user=y3JNIdsAAAAJ&hl=en>**EMPLOYMENT**

- | | |
|---|-----------------------------------|
| 1. Associate Professor , ASU at the Polytechnic campus, Mesa, AZ | <i>May 2014 – present</i> |
| Graduate Faculty , Department of Physics, ASU, Tempe | <i>October 2008 – present</i> |
| Graduate Faculty , Materials Sciences, ASU, Tempe | <i>February 2012 – present</i> |
| Graduate Faculty , SMACS Program, ASU, Polytechnic | <i>May 2011 - present</i> |
| Graduate Faculty , Systems Engineering, ASU, Polytechnic/Tempe | <i>Aug 2018 - present</i> |
| 2. Assistant Professor , ASU at the Polytechnic campus, Mesa, AZ | <i>August 2008 – May 2014</i> |
| 3. Postdoctoral Researcher , RPI, Troy, NY | <i>October 2007 – August 2008</i> |
| 4. Visiting Assistant Professor , Skidmore College, NY | <i>September 2007 – May 2008</i> |
| 5. Research Consultant , General Electric, Global Research, NY | <i>May 2005 – December 2005</i> |
| 6. Research Intern , GE, Global Research Center, NY | <i>May 2004 – August 2004</i> |

EDUCATION**Rensselaer Polytechnic Institute (RPI)**, Troy, New York, USA**Ph. D. in Physics, 2007****Beijing Normal University**, Beijing, China**B. S. in Physics, 2000****PROFESSIONAL AFFILIATIONS**

1. The American Physical Society, USA - Member since 2006.
2. The American Chemical Society, USA - Member since 2012.
3. Sigma Pi Sigma Honor Society, USA - Member since 2005.

KEY RESEARCH INTERESTS

- First-principle density-functional theory calculations of electronic properties, strain effect and photo-chemical characteristics of group IV, V, III-V, II-VI nanowires, carbon nanotubes, graphene nanoribbons and phosphorene for potential application in nano-electronic devices.
- Investigation of novel materials for photocatalysts and high capacity Li-ion battery electrodes through theoretical calculations.
- Investigation of physical and photo-chemical properties of transition metal oxide catalysts via density-functional theory.

I. SCHOLARLY ACTIVITIES

A. PUBLICATIONS

The **advised students** are underlined and in bold, and the advised visiting scholar is denoted using †, and the corresponding authors are denoted using *.

A1. Book Chapters

1. **X.-H. Peng***, **A. Copple**, Q. Wei†, “Strain Engineered Direct-indirect Band Gap Transition and its Mechanism in 2D Phosphorene”, *Computational and Theoretical Nanoscience of Two-Dimensional Materials*, Xiaobin Niu & Zhiming Wang (Editors), 2017. Springer. In press. (Invited book chapter)
2. **X.-H. Peng***, F. Tang, **P. Logan**, “Electronic properties of Si and Ge nanowires, a first-principles study”, *Handbook of Nanomaterials Properties*, Bharat Bhushan (Editor), 2014, page 51-83. Springer. http://link.springer.com/chapter/10.1007/978-3-642-31107-9_26
3. **X.-H. Peng***, F. Tang, **P. Logan**, “First principles study of Si/Ge core-shell nanowires – Structural and Electronic Properties”, *Chapter 4, Nanowires – Fundamental Research*, Abbass Hashim (Editor), 2011 In Tech. <http://www.intechopen.com/books/nanowires-fundamental-research>
4. 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.

A2. Peer-Reviewed Journal Articles

Under review:

1. **Andrew Dopilka**, Ran Zhao, J. Mark Weller, Svilen Bobev, **Xihong Peng**, Candace K. Chan*, “Experimental and Computational Study of the Lithiation of Ba₈Al_yGe_{46-y} Based Type I Germanium Clathrates”, *ACS Applied Materials & Interfaces*, under review.

Published:

2. **Guang Yang**†, Tianxing Ma*, and **Xihong Peng***, “Superior mechanical flexibility and strained-engineered direct-indirect band gap transition of green phosphorene”, *Applied Physics Letters* **112**, 241904 (2018).
3. Kwai S. Chan*, Michael A. Miller, **Xihong Peng**, “First-Principles Computational Study of Hydrogen Storage in Silicon Clathrates”, *Materials Research Letters* **6 (1)**, 72-78 (2018). DOI: 10.1080/21663831.2017.1396261 (Published online Nov. 02, 2017)
4. Kwai S. Chan*, **Xihong Peng**, “First-Principles Study of the Electronic Structure of Type I Hybrid Carbon-Silicon Clathrates”, *Journal of Electronic Materials* **45 (8)**, 4246-4255. DOI 10.1007/s11664-016-4621-3 (2016)
5. **Xihong Peng**, Qun Wei†, Ying Li, Candace Chan* “First principles study of lithiation of type I Ba-doped silicon clathrates”, *Journal of Physical Chemistry C* **119(51)**, 28247-28257. (2015).

6. **A. Arvay, I. French, J.-C. Wang, X.-H. Peng** and A.M. Kannan*, “Modeling and simulation of biologically inspired flow field designs for proton exchange membrane fuel cells”, *The Open Electrochemistry Journal* **6**, 1-9. (2015)
7. **Xihong Peng**, Man Li, Candace Chan* “Investigation of the optical absorbance, electronic, and photocatalytic properties of $(\text{Cu}_{1-x}\text{Co}_x)_2(\text{OH})\text{PO}_4$ solid solutions”, *Journal of Physical Chemistry C* **119**, 4684-4693. (2015).
8. Zhigang Liu*, Zili Wu, **Xihong Peng**, Andrew Binder, Songhai Chai, Sheng Dai, “Origin of active oxygen in a ternary $\text{CuO}_x/\text{Co}_3\text{O}_4\text{-CeO}_2$ catalyst for CO oxidation”, *Journal of Physical Chemistry C* **118**, 27870-27877 (2014).
9. **Xihong Peng***, Qun Wei†, “Chemical scissors cut phosphorene nanostructures”, *Materials Research Express* **1**, 045041 (2014).
10. **Xihong Peng***, **Andrew Copple**, Qun Wei†, “Edge effects on the electronic properties of phosphorene nanoribbons”, *Journal of Applied Physics* **116**, 144301 (2014).
11. **Xihong Peng***, Qun Wei†, **Andrew Copple**, “Strain engineered direct-indirect band gap transition and its mechanism in 2D phosphorene”, *Physical Review B* **90**, 085402 (2014).
12. Qun Wei†, **Xihong Peng***, “Superior mechanical flexibility of phosphorene and few-layer black phosphorus”, *Applied Physics Letters* **104**, 251915 (2014).
13. Nicholas A. Wagner, Rahul Raghavan, Ran Zhao, Qun Wei†, **Xihong Peng**, Candace K. Chan*, “Electrochemical cycling of sodium-filled silicon clathrate”, *ChemElectroChem* Volume 1, Issue 2, pages 347-353, (2014).
14. M. Li, Q. Cheng, R. M. Wittman, **X.-H. Peng** and C. K. Chan*, “Electrochemical and Photoelectrochemical Properties of the Copper Hydroxyphosphate Mineral Libethenite”, *ChemElectroChem*, Volume 1, Issue 3, pages 663-672, (2014).
15. Kwai S. Chan*, Michael A. Miller, Wuwei Liang, Carol Ellis-Terrell, and **Xihong Peng**, “First principles computational design and synthesis of hybrid carbon-silicon clathrates”, *Journal of Materials Science* **49**, 2723-2733 (2014).
16. **X.-H. Peng***, **A. Copple**, “Origination of the direct-indirect band gap transition in strained wurtzite and zinc-blende GaAs nanowires: a first principles study”, *Physical Review B* **87**, 115308 (2013).
17. **A. Arvay, I. French, J.-C. Wang, X.-H. Peng** and A. M. Kannan*, “Nature inspired flow field designs for proton exchange membrane fuel cell”, *International Journal of Hydrogen Energy* **38**, 3717-3726 (2013).

18. Q. Cheng, **X.-H. Peng**, C. K. Chan*, “Structural and photoelectrochemical evaluation of nanotextured Sn-doped AgInS₂ films prepared by spray pyrolysis”, *ChemSusChem* **6** (1), 102-109 (2013).
19. **A. Copple**, **N. Ralston**, **X.-H. Peng***, “Engineering direct-indirect band gap transition in wurtzite GaAs nanowires through size and uniaxial strain”, *Applied Physics Letters* **100**, 193108 (2012).
20. **X.-H. Peng***, F. Tang, **A. Copple**, “Engineering the work function of armchair graphene nanoribbons using strain and surface functional species: a first principles study”, *Journal of Physics: Condensed Matter* **24**, 075501(2012).
21. M. M. Rodriguez, **X.-H. Peng**, L. Liu, Y. Li, and J. M. Andino*, “A density functional theory and experimental study of CO₂ interaction with brookite TiO₂”, *The Journal of Physical Chemistry C* **116** (37), 19755-19764 (2012).
22. **A. Arvay**, E. Yli-Rantala, C.-H. Liu, **X.-H. Peng**, P. Koski, L. Cindrella, P. Kauranen, P. M. Wilde, and A. M. Kannan*, “Characterization techniques for gas diffusion layers for proton exchange membrane fuel cells – a review”, *Journal of Power Sources* **213**, 317-337 (2012).
23. **A. Arvay**, **A. Ahmed**, **X.-H. Peng**, A. M. Kannan*, “Convergence criteria establishment for 3D simulation of proton exchange membrane fuel cell”, *International Journal of Hydrogen Energy* **37**, 2482-2489 (2012).
24. **X.-H. Peng***, F. Tang, **P. Logan**, “Band structure of Si/Ge core-shell nanowires along the [110] direction modulated by external uniaxial strain”, *Journal of Physics: Condensed Matter* **23**, 115502 (2011).
25. **X.-H. Peng***, **S. Velasquez**, “Strain modulated band gap of edge passivated armchair graphene nanoribbons”, *Applied Physics Letters* **98**, 023112 (2011).
26. **X.-H. Peng***, **P. Logan**, “Electronic properties of strained Si/Ge core-shell nanowires” *Applied Physics Letters* **96**, 143119 (2010).
27. J. F. Lin, C. W. Mason, A. Adame, X. Liu, **X.-H. Peng**, A. M. Kannan*, “Synthesis of Pt nanocatalyst with micelle-encapsulated multi-walled carbon nanotubes as support for proton exchange membrane fuel cells”, *Electrochimica Acta* **55**, 6496-6500 (2010).
28. **P. Logan**, **X.-H. Peng***, “Strain-modulated electronic properties of Ge nanowires: a first-principles study”, *Physical Review B* **80**, 115322 (2009).
29. **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”, *International Journal of Applied Mechanics* **1**, 483 (2009).

30. Y. Zhang, **X.-H. Peng**, Y. Chen, A. Curino, W. Andreoni, S. K. Nayak*, X.-C. Zhang, and “A first principle study of terahertz (THz) spectra of acephate”, *Chemical Physics Letters* **452**, 59-66 (2008).
31. S. Sreekala*, **X.-H. Peng**, P. M. Ajayan, and S. K. Nayak, “Effect of strain on the band gap and effective mass of zigzag single-wall carbon nanotubes: first-principles density-functional calculations”, *Physical Review B* **77**, 155434 (2008).
32. **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”, *Journal of Applied Physics* **102**, 024304 (2007).
33. **X.-H. Peng***, A. Alizadeh, N. Bhate, K. K. Varanasi, S. K. Kumar, and S. K. Nayak, “First-principles investigation of strain effects on the energy gaps in Si nanoclusters”, *Journal of Physics: Condensed Matter* **19**, 266212 (2007).
34. **X.-H. Peng***, S. Ganti, A. Alizadeh, P. Sharma, S. K. Kumar, and S. K. Nayak, “Strain-engineered photoluminescence of silicon nanoclusters”, *Physical Review B* **74**, 035339 (2006).
35. 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”, *Physical Review B* **73**, 035413 (2006).
36. **X.-H. Peng**, S. Ganti, P. Sharma*, A. Alizadeh, S. K. Nayak, S. K. Kumar, “Novel scaling laws for band gaps of quantum dots”, *Journal of Computational and Theoretical Nanoscience* **2**, 469 (2005).
37. 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”, *Physical Review Letters* **93**, 188301 (2004).
38. M. Zhan*, Z.-G. Zheng, G. Hu, **X.-H. Peng**, “Nonlocal chaotic phase synchronization”, *Physical Review E* **62**, 3552 (2000).

B. PRESENTATION

B1. Conference Presentations

The presenters are denoted using *, the **advised students** are underlined and in bold, and the advised visiting scholar is denoted using †.

1. **X.-H. Peng***, Q. Wei†, **A. Copple**, “Strain engineered direct-indirect band gap transition and its mechanism in 2D phosphorene”, American Physical Society (APS), 2016 March (international) meeting, Baltimore, MD (Poster presentation, March 15th, 2016).
2. **X.-H. Peng***, Q. Wei†, “Chemical scissors cut phosphorene and their novel electronic properties”, American Physical Society (APS), 2015 March (international) meeting, San Antonio, TX (Oral presentation, March 3rd, 2015).

3. **X.-H. Peng***, **A. Copple**, Q. Wei†, “Size and strain dependence of electronic properties in ultrathin ZnO nanowires”, American Physical Society (APS), 2014 March (international) meeting, Denver, CO (Oral presentation, March 3rd, 2014).
4. **X.-H. Peng***, **A. Copple**, **N. Ralston**, “Strain manipulated direct-indirect band gap transition in GaAs nanowires”, American Physical Society (APS), 2013 March (international) meeting, Baltimore, MD (Oral presentation, March 18th, 2013).
5. **A. Copple***, **N. Ralston**, **X.-H. Peng**, “Engineering direct-indirect band gap transition in wurtzite GaAs nanowires through size and uniaxial strain”, APS, 2012 4-Corners-Section (regional) meeting, Socorro, NM (Oral presentation, October 27th, 2012).
6. **S. Caudle***, M. Tao, **X.-H. Peng**, “First-principles study of transition metal (TM=Pb, Cu) oxides/sulfides”, APS, 2012 4-Corners-Section (regional) meeting, Socorro, NM (Oral presentation, October 26th, 2012).
7. **X.-H. Peng***, F. Tang, **S. Velasquez**, and **A. Copple**, “Engineering electronic properties of armchair graphene nanoribbons using strain and functional species”, APS, 2012 March (international) meeting, Boston, MA (Oral presentation, February 29th, 2012).
8. **X.-H. Peng***, F. Tang, **P. Logan**, “Electronic properties of strained Si/Ge core-shell nanowires”, International Symposium on Clusters and Nano-Structures (ISCAN), Richmond, VA (Poster presentation, November 7th, 2011).
9. **A. Copple***, **X.-H. Peng**, **S. Velasquez**, F. Tang, “Tunable electronic properties of armchair graphene nanoribbons from first-principles calculations”, APS, 2011 4-Corners-Section (regional) meeting, Tucson, AZ (Poster presentation, October 21st, 2011).
10. **A. Copple**, **N. Ralston***, **P. Nguyen**, **X.-H. Peng**, “*Ab initio* study of wurtzite InAs and GaAs nanowires”, APS, 2011 4-Corners-Section (regional) meeting, Tucson, AZ (Poster presentation, October 21st, 2011).
11. **K. Ashe***, **X.-H. Peng**, “Strain-modulated Fermi velocity of charge carriers in 2D graphene: A first principles study”, APS, 2011 4-Corners-Section (regional) meeting, Tucson, AZ (Poster presentation, October 21st, 2011).
12. **X.-H. Peng***, **P. Logan**, “First principles study of Si/Ge core-shell nanowires along [110] direction”, APS, 2011 March (international) meeting, Dallas, TX (Oral presentation, March 24th, 2011).
13. **P. Logan***, **X.-H. Peng**, “Electronic properties of strained Si [111] nanowires”, APS, 2010 March (international) meeting, Portland, OR (Poster presentation, March 15th, 2010).
14. **P. Logan***, **X.-H. Peng**, “Quantum confinement in strained Si/Ge core-shell nanowires”, APS, 2009 4-Corners-Section (regional) meeting, Golden, CO (Poster presentation, October 23rd, 2009, won the “*Best Paper Award*”).

15. **S. Velasquez***, **P. Logan**, **X.-H. Peng**, "Strain and edge passivation induced band gap modulation and effective mass tuning in armchair graphene nanoribbons", APS, 2009 4-Corners-Section (regional) meeting, Golden, CO (Poster presentation, October 23rd, 2009).
16. **P. Logan**, **X.-H. Peng***, "The effects of strain and quantum confinement on the electronic properties of germanium nanowires", APS, 2009 March (international) meeting, Pittsburgh, PA (Oral presentation, March 17th, 2009).
17. **X.-H. Peng***, J. Anderson, G. Tepper, S. Bandyopadhyay, S. Nayak, "Quantum confined Stark effect in organic fluorophores", APS, 2008 March (international) meeting, New Orleans, LA (Oral presentation, March 14th, 2008).
18. **X.-H. Peng***, S. K. Kumar, S. K. Nayak, "First principles study of strain effects on the electronic properties in silicon nanowires", APS, 2007 March (international) meeting, Denver, CO (Oral presentation, March 9th, 2007).
19. 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", APS, 2007 March (international) meeting, Denver, CO (Oral presentation, March 8th, 2007).
20. **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", APS, 2006 March (international) meeting, Baltimore, MD (Oral presentation, March 13th, 2006).
21. **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", APS, 2006 March (international) meeting, Baltimore, MD (Poster presentation, March 14th, 2006).
22. 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 (international) meeting, Austin, TX (Oral presentation, November 2004).
23. N. Adhikari*, **X.-H. Peng**, S. K. Nayak, S. K. Kumar, "Modeling the surfactant mediated synthesis of quantum nanodots and their arrays", APS, 2004 March (international) meeting, Montreal, Quebec, Canada (Oral presentation, March 2004).

B2. ASU Presentations and Exhibits

1. **A. Copple***, **X.-H. Peng**, **S. Velasquez**, "Tunable electronic properties of armchair graphene nanoribbons from first-principles calculations" at the College of Technology and Innovation Showcase (Poster presentation, April 25th, 2012).
2. **A. Copple***, **X.-H. Peng**, **S. Velasquez**, "Tunable electronic properties of armchair graphene nanoribbons from first-principles calculations" at the College of Technology and Innovation event of "Thing on Thursday" Mini Innovation Showcase (Poster presentation, September 8th, 2011).

3. **A. Copple, N. Ralston,* X.-H. Peng**, “Ab Initio study of wurtzite InAs and GaAs nanowires” at the College of Technology and Innovation event of “Thing on Thursday” Mini Innovation Showcase (Poster presentation, September 8th, 2011).
4. **X.-H. Peng*, P. Logan, F. Tang, S. Velasquez**, “Tunable electronic properties from semiconductor nanostructures” at the College of Technology and Innovation event of “Thing on Thursday” Mini Innovation Showcase (Poster presentation, September 8th, 2011).
5. **X.-H. Peng*, P. Logan, F. Tang, S. Velasquez**, “Tunable electronic properties from semiconductor nanostructures” at the College of Technology and Innovation Showcase (Poster presentation, May 5th, 2011).
6. **X.-H. Peng, P. Logan*, S. Velasquez**, “Tunable luminescence from semiconductor nanostructures” at the ASU Polytechnic Campus “Earth Day” Festival (Poster presentation, April 18th, 2009).

C. RESEARCH GRANTS AND RESOURCES

C1. Awards and Sponsored Research Grants

1. Funded by National Science Foundation (NSF), Division of Materials Research
“Collaborative Research: Synthesis, Structural Characterization and Electrochemical Studies of Framework Substituted Germanium and Tin Clathrates”
Funding period: September 1, 2017 – August 31, 2020
Award amount: \$195,000
Role: Co-PI (PI: Candace Chan; Co-PI: Xihong Peng)
Peng’s share: 50%
2. Funded by National Science Foundation (NSF), Division of Undergraduate Education
“Identifying and addressing mathematical difficulties in introductory physics courses”
Funding period: September 1, 2015 – August 31, 2019
Award amount: \$250,000
Role: Co-PI (PI: David Meltzer; Co-PIs: Yun Kang & Xihong Peng)
Peng’s share: 29%
3. Funded by Arizona ABOR, Materials Research Seed Initiative
“Tri-University Advanced Materials Project, at the interface: hybrid materials leading to new energy conversion and energy storage platforms”
Funding period: January 1, 2015 – June 30, 2016
Award amount: \$200,000
Role: Senior Personnel (ASU PI: Robert Nemanich; UA PI Neal Armstrong; NAU PI Constantin Ciocanel)
Peng’s share: supported a Graduate Research Assistantship and additional \$2000 to purchase computing hours from ASU computing center.

4. Funded by School of Letters and Sciences, Arizona State University
 “Development of novel materials/catalysts for applications in alternative renewable energies – preliminary data collection”
 Funding period: Summer 2013
 Award amount: \$15,000
 Role: PI
 Peng’s share: 100%
5. Funded by Salt River Project
 “Reliability and performance evaluation of batteries in hot/dry climate”
 Funding period: 6/15/2012 – 6/30/2013
 Award amount: \$44,938
 Role: Co-PI
 Peng’s share: 25%
6. Funded by School of Letters and Sciences, Arizona State University
 “Earth-abundant metal oxysulfides as active layer in next-generation photovoltaics – preliminary data collection”
 Funding period: 1/1/2013 – 6/30/2013
 Award amount: \$14,714
 Role: PI
 Peng’s share: 100%
7. Funded by College of Technology and Innovation, Arizona State University
 “Synthesis effects of catalytic defect and strain in hydrogenation/dehydrogenation of MgH₂ – preliminary data collection”
 Funding period: 2/1/2011 – 6/15/2011
 Award amount: \$16,951
 Role: PI
 Peng’s share: 70%

C2. Computing Resources Awarded

#	My role	Topic	Computing Resources	Resource Awarded (cpu-hour)	Duration
1	PI	III-V nanowires	XSEDE, NSF	200,000	9/2013-9/2014
2	PI	Battery materials	ASU(Saguaro)	106,000	5/2012-5/2013
3	PI	PV materials	ASU(Saguaro)	45,000	1/2012-1/2013
4	PI	High-K materials	ASU(Saguaro)	160,000	8/2011-8/2012

5	PI	III-V nanowires	ASU(Saguaro)	115,000	5/2011-5/2012
6	PI	PEM fuel cells	ASU(Saguaro)	40,000	8/2010-8/2011
7	PI	Graphene	ASU(Saguaro)	94,000	3/2010-3/2011
8	PI	Ge nanowires	Teragrid-PSC (bigBen, Pople)	140,000	10/2008-10/2009
9	PI	Core-shell nanowires	Teragrid-NCSA (Abe, Cobalt)	60,000	10/2008-10/2009

D. COLLOQUIUM AND SEMINAR TALKS

1. **(Invited)** “Materials research for applications in nano-electronics and renewable energies using first-principles computation”, Physics Department, Jiangnan University, Wuhan, China, May 4th, 2018.
2. “Computational materials research for applications in nano-electronics and renewable energies”, Science and Mathematics Seminar, College of Integrative Sciences and Arts, Arizona State University, August 31st, 2016.
3. **(Invited)** “Computational materials research and applications in nano-electronics and renewable energies”, Guangzhou Institute of Geochemistry, Chinese Academy of Science, Guangzhou, China, June 4th, 2015.
4. **(Invited)** “Frontier research of material sciences from the aspect of computational physics and chemistry”, Chemistry Department, Hunan University, Changsha, China, May 28th, 2015.
5. **(Invited)** “Computational materials research and applications in nano-electronics and renewable energies”, Chemistry Department, Hunan University, Changsha, China, June 9th, 2014.
6. “Computational materials research for applications in nano-electronics and renewable energies”, Science and Mathematics Seminar, School of Letters and Sciences, Mesa, AZ, August 28th, 2013.
7. **(Invited)** “Strain engineered electronic properties in semiconductor nanostructures”, Physics Department, Washington University in St. Louis, St. Louis, MO, February 25th, 2013.
8. **(Invited)** “Energy gaps and quantum carriers in strained nanostructures”, College of Nanoscale Science and Engineering, University at Albany, State University of New York, Albany, NY, February 21st, 2013.
9. **(Invited)** “Energy gaps and quantum carriers in strained nanostructures”, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY, February 20th, 2013.

10. **(Invited)** “Predictive modeling for nanoscale system using first-principles calculations: Structural and electronic”, Department of Physics, California State University in Fresno, Fresno, CA, October 12th, 2012.
11. **(Invited)** “Predictive modeling for nanoscale system using first-principles calculations”, Beijing Computational Science Research Center, Beijing, China, May 24th, 2012.
12. “Predictive modeling for nanoscale system using first principles calculation: - structural, electronic and catalytic properties”, SMACS (Simulation, Modeling, and Applied Cognitive Science) Program Seminar, Arizona State University at Polytechnic Campus, Mesa, AZ, March 7th, 2012.
13. “Predictive modeling for nanoscale system using first principles calculation: - its application to photovoltaic materials”, AISES (American Indian Science and Engineering Society) Program Seminar, Arizona State University, Tempe, AZ, February 16th, 2012.
14. “Predictive modeling for nanoscale system using first principles calculation: - structural, electronic and catalytic properties”, Department of Applied Sciences and Mathematics, Arizona State University at Polytechnic Campus, Mesa, AZ, August 30th, 2011.
15. **(Invited)** “Predictive modeling for nanoscale materials using first principles calculation: - photoluminescence of quantum dots and Stark effect in fluorescent molecules”, Department of Mechanical Engineering, University of Houston, Houston, TX, May 21st, 2009.
16. “Predictive modeling for nanoscale materials using first principles calculation”, Department of Physics, Arizona State University, Tempe, AZ, November 10th, 2008.
17. **(Invited)** “Tunable luminescence from silicon quantum dots”, Department of Physics, University of Massachusetts, Dartmouth, MA, March 27th, 2008.
18. **(Invited)** “Tunable luminescence from silicon quantum dots”, Department of Physics, University of Wisconsin-Eau Claire, Eau Claire, WI, March 11th, 2008.
19. **(Invited)** “Tunable luminescence from silicon quantum dots”, Department of Physics, Westminster College, Fulton, MO, February 6th, 2008.
20. **(Invited)** “Tunable luminescence from silicon quantum dots”, Department of Physics, Skidmore College, Saratoga Springs, NY, April 5th, 2007.
21. “Silicon quantum dots”, Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, Troy, NY, July 19th, 2006.

E. OTHER PROFESSIONAL/SCHOLARLY ACTIVITIES

1. **Invited Visiting Professor** in Department of Physics, Jiangnan University, Wuhan, China during the period of April 27 – May 5, 2018. Worked on a collaborative training program to graduate students with Profs. X.-L. Zhu and Y. Tian.
2. **Visiting Professor** in Wuhan University. As one of four core faculty, participated in a four-week program led by the ASU President's office, Director of China Affair, to build ties with Wuhan University by delivering workshop lectures at Wuhan, China during the period of May 18th – June 12th, 2015. Each of our four participating faculty delivered two courses to enhance professional development around research/publication issues for the graduate students at Wuhan University and received excellent feedback from both students and administrative sides of Wuhan University.
3. **Invited Visiting Professor** in Beijing Computational Science Research Center, Beijing, China during the period of May 20th – 27th, 2012, where I worked on a collaborative project on magnetic properties of graphene with Prof. T.-X. Ma.
4. **Visiting Professor** in Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, Troy, NY during the period of June 14th – 27th, 2009, where I worked on a project on strained graphene sheets in collaboration with Prof. S.K. Nayak.
5. **Visiting Professor** in Department of Mechanical Engineering, University of Houston, Houston, TX during May 19th – 25th, 2009, where I helped to train Prof. P. Sharma's research group using the density functional simulation tool VASP and participated in a project on nanoscale capacitors.

II. INSTRUCTIONAL ACTIVITIES**F. CLASSROOM TEACHING**

Year	Term	Course	Title	Credit Hours	Enrollment
2018	Fall	PHY 792	Graduate Research	6	1
2018	Fall	PHY 121	University Physics I: Mechanics	3	56
2018	Fall	PHY 321	Vector Mechanics and Vibration	3	14
2018	Summer	PHY792	Graduate Research	6	1
2018	Spring	PHY500	Graduate Research Rotation	3	1
2018	Spring	PHY 252	Physics III	4	3
2018	Spring	PHY 321	Vector Mechanics and Vibration	3	31
2017	Fall	PHY 111	General Physics I	3	16
2017	Fall	PHY 321	Vector Mechanics and Vibration	3	37
2017	Spring	PHY 112	General Physics II	3	16
2017	Spring	PHY 321	Vector Mechanics and Vibration	3	22

2016	Fall	PHY 112	General Physics II	3	52
2016	Fall	PHY 321	Vector Mechanics and Vibration	3	36
2016	Spring	PHY 131	University Physics II	3	35
2016	Spring	PHY 321	Vector Mechanics and Vibration	3	20
2015	Spring	PHY 131	University Physics II	3	24
2015	Spring	PHY 321	Vector Mechanics and Vibration	3	60
2015	Spring	PHY 792	Graduate Research	9	1
2014	Fall	PHY 111	General Physics I	3	68
2014	Fall	PHY 112	General Physics II	3	40
2014	Fall	PHY 792	Graduate Research	9	1
2014	Spring	PHY 111	General Physics I	3	87
2014	Spring	PHY 321	Vector Mechanics and Vibration	3	27
2014	Spring	PHY 792	Graduate Research	9	1
2013	Fall	PHY 112	General Physics II	3	64
2013	Fall	PHY 321	Vector Mechanics and Vibration	3	58
2013	Fall	PHY 792	Graduate Research	9	1
2013	Summer	PHY 792	Graduate Research	1	1
2013	Spring	PHY 111	General Physics I	3	85
2013	Spring	PHY 792	Graduate Research	6	2
2012	Fall	PHY 112	General Physics II	3	63
2012	Fall	PHY 321	Vector Mechanics and Vibration	3	52
2012	Fall	PHY 792	Graduate Research	6	2
2012	Summer	PHY 792	Graduate Research	6	2
2012	Spring	PHY 112	General Physics II	3	94
2012	Spring	PHY 792	Graduate Research	6	2
2012	Spring	PHY 500	Graduate Research Rotation	3	1
2011	Fall	PHY 112	General Physics II	3	68
2011	Fall	PHY 321	Vector Mechanics and Vibration	3	30
2011	Fall	ABS 498	Undergraduate Research	3	1
2011	Fall	PHY 792	Graduate Research	6	1
2011	Summer	PHY 792	Graduate Research	3	2
2011	Spring	PHY 112	General Physics II	3	52
2011	Spring	PHY 112	General Physics II (Lab)	3	20
2011	Spring	PHY 111	General Physics I (Recitation)	1	24
2011	Spring	ABS 489	Undergraduate Research	3	1
2010	Fall	PHY 112	General Physics II	3	58
2010	Fall	PHY 321	Vector Mechanics and Vibration	3	24
2010	Fall	EGR 401	CTI Capstone Projects I	4	7
2010	Fall	PHY 500	Graduate Research Rotation	3	1
2010	Summer	PHY 792	Graduate Research	3	1

2010	Summer	ABS 489	Undergraduate Research	1	1
2010	Spring	PHY 112	General Physics II	3	56
2010	Spring	PHY 112	General Physics II	3	27
2010	Spring	PHY 792	Graduate Research	9	1
2010	Spring	ABS 489	Undergraduate Research	2	1
2010	Spring	ABS 499	Individualized Instruction	1	1
2009	Fall	PHY 111	General Physics I	3	68
2009	Fall	PHY 112	General Physics II	3	63
2009	Fall	PHY 792	Graduate Research	5	1
2009	Fall	ABS 499	Individualized Instruction	3	1
2009	Summer	ABS 499	Individualized Instruction	3	1
2009	Spring	PHY 112	General Physics II	3	62
2009	Spring	PHY 112	General Physics II	3	25
2009	Spring	PHY 792	Graduate Research	6	1
2009	Spring	ABS 489	Undergraduate Research	1	2
2008	Fall	PHY 111	General Physics I	3	48
2008	Fall	PHY 112	General Physics II	3	45
2008	Fall	PHY 112	General Physics II-Recitation	1	25

G. MENTORING

a. Graduate Students

Graduate Student's Award: One of my mentored students, Paul Logan, received the "*Best Paper Award*" at the American Physical Society 4-Corners Sectional Conference for his poster presentation (October 2009).

a) **As a Committee Chair**

- 1) Ph.D. student Andrew Copple (ASU, Tempe, Physics Department) on the dissertation of "Tuning the Electronic Properties of Nanoscale Semiconductors" and received the Ph.D. in Physics in August 2016.
- 2) Master student Sean Caudle (ASU, Tempe, Physics Department) on the project of "Earth abundant photovoltaic materials", and received the MS degree in Nanoscience in Dec. 2013.
- 3) Master student Andrew Copple (ASU, Tempe, Physics Department) on the projects of "Strain effects on the edge passivated graphene nanoribbons" and received the Master Degree of Science (MS) degree in Physics in May 2012.
- 4) Master student Nathaniel Ralston (ASU, Tempe, Physics Department) on the projects of "III-V nanowires" and received the MS in Physics in May 2012.

- 5) Ph.D. student Paul Logan (ASU, Tempe, Physics Department) on the project of “Group IV semiconductor nanowires”. Spring 2009-summer 2000.

b) As a Committee Co-Chair

- 6) Ph.D. student Xuan Shi (ASU, Polytechnic, Systems Engineering Program) on the project of PEM fuel cells, Spring 2018 – present.
- 7) Master student Abshir Ahmed (ASU, Polytechnic, Engineering Department) on the applied project titled “Mesh sensitivity analysis for proton exchange membrane fuel cells” and received the MS degree in Technology in December 2011.
- 8) Ph.D. student Adam Arvay (ASU, Polytechnic, Engineering Department) on the project of “Nature-inspired flow field design in PEM fuel cells”. 2011-2014
- 9) Master student Jui-Chieh Wang (ASU, Polytechnic, Engineering Department) on the project of “PEM fuel cell flow field design”. 2011

c) As a Committee Member

- 10) Master student Mathan Moorthy (ASU, Polytechnic, Engineering Department) on the project of “fuel cells”, MS degree in Technology in May 2015.
- 11) Ph.D. student Jialing Yang (ASU, Tempe, Physics Department) on the thesis titled “Interface electronic state characterization of remote plasma enhanced atomic layer deposition high-k/low-k dielectric on GaN”, and received the Ph.D. in Physics in May 2014.
- 12) Master student Sri Harsha Kolli (ASU, Polytechnic, Engineering Department) on the project of “Potential materials for fuel cells”, and received the MS degree in Technology in Dec. 2014.
- 13) Master student Ben Folsom, (ASU, Tempe, Physics Department) on the project of “Carbon pillars and metallic nanoframes: a density functional theory study”, and received the MS degree in Nanoscience in May 2014.
- 14) Master student Prashanth Ganeshram (ASU, Polytechnic, Engineering Department) on the project of “Impedance measurement of batteries”, and received the MS degree in Technology in May 2014.

- 15) Ph.D. student Tianyin Sun (ASU, Tempe, Physics Department) on the thesis titled “Combined photo- and thermionic electron emission from low work function diamond films”, and received the Ph.D. in Physics in December 2013.
- 16) Master student Maxx Patterson (ASU, Polytechnic, Engineering Department) on the thesis titled “A study of PV, batteries and fuel cells system based hybrid micro-grid model for intermittent community services” and received the MS degree in Technology in May 2013.
- 17) Ph.D. student Xinyang Wang (ASU, Tempe, Physics Department) on the thesis titled “Relativistic matter under extreme conditions”, and received the Ph.D. in Physics in summer 2013.
- 18) Master student Ximo Chu (ASU, Polytechnic, Engineering Department) on the project of “Characterization of batteries”, and received the MS degree in Technology in December 2013.
- 19) Master student Jason French (ASU, Polytechnic, Engineering Department) on the applied project titled “Modeling and simulation of bio-inspired flow field designs for proton-exchange membrane fuel cells” and received the MS degree in Technology in December 2012.
- 20) Master student Yen Huang (ASU, Polytechnic, Engineering Department) on the applied project titled “Synthesis of single walled carbon nanotubes” and received the MS degree in Technology in December 2012.
- 21) Master student Anthony Adame (ASU, Polytechnic, Engineering Department) on the thesis titled “Development of platinum-copper core-shell nanocatalyst on multi-walled carbon nanotubes for proton exchange membrane fuel cells” and received the MS degree in Technology in May 2012.
- 22) Master student Rashida Villacorta (ASU, Polytechnic, Engineering Department) on the thesis titled “Graphene based gas diffusion layers for use in fuel cells and hydrogen storage” and received the MS degree in Technology in May 2012.
- 23) Master student Aditi Jhalani (ASU, Polytechnic, Engineering Department) on the applied project titled “Porphyrin group as cathode catalyst for alkaline fuel cells” and received the MS degree in Technology in May 2012.
- 24) Ph.D. student Sourabh Sinha (ASU, Tempe, Physics Department) on the thesis titled “Models for amorphous calcium carbonate” and received the Ph.D. in Physics in December 2011.

- 25) Master student Kartik Kinhal (ASU, Polytechnic, Engineering Department) on the thesis titled "Effects of sputtered platinum counter electrode and integrated TiO₂ electrode with SWCNT on DSSC performance" and received the MS degree in Technology in December 2011.
- 26) Master student Adam Arvay (ASU, Polytechnic, Engineering Department) on the thesis titled "Proton exchange membrane fuel cell modeling and simulation using Ansys Fluent" and received the MS degree in Technology in May 2011.

d) As a Research Rotation Project Adviser for Physics Graduate Students

- 1) Evan Garrison (spring 2018, "size effect of green phosphorene nanoribbons")
- 2) Andrew Copple (fall 2010, "edge effects of graphene nanoribbons")
- 3) Nathaniel Ralston (fall 2011, "quantum confinement effect of group III-V nanowires")
- 4) Sean Caudle (fall 2012, "electronic properties of photovoltaic materials")

e) As a Faculty mentor for the Program of U.S. - Pakistan Center for Advanced Studies in Energy (USPCAS-E) for the following Pakistan graduate visiting scholars

- 5) Afaf Ali from University of Engineering and Technology (UET), Peshawar, Pakistan. (fall 2018, PEM fuel cells)
- 6) Shahbaz Ahmad from UET, Peshawar, Pakistan. (fall 2018, PEM fuel cells)
- 7) Wajeha Taugir from National University of Science and Technology (NUST), Islamabad, Pakistan. (fall 2018, Solar thermal space heating)
- 8) Ihtesham Ahmad from NUST, Islamabad, Pakistan. (fall 2018, batteries)
- 9) Muhammad Arif from NUST, Islamabad, Pakistan. (fall 2018, batteries)

b. Undergraduate Students

Student's awards: One of my mentored undergraduate students, Selina Velasquez, won the "***Undergraduate Research Award***" in April 2010 from the Department of Applied Sciences and Mathematics for her excellent work completed in my group.

a) Barret Honors thesis

1. Matthew Jones, Barret Honors Thesis. As a Co-advisor of his thesis. Thesis title "*The Mathematical Successes and Failures of Students in an Introductory Physics Course*", defended 11/24/2016.
2. Tom Nagy. Served as committee member of the honor's thesis titled "Hands-on laser lab for undergraduate students: developing and assessment", defended 11/30/2012.

b) Barret Honors project

3. Alexander Gavrillov, Barret Honors Project contracted with PHY121 course in fall 2018. Project topic "mechanical properties of Si/Ge clathrates".

4. Jacob Tanaka, Barret Honors Project contracted with PHY121 course in fall 2018. Project topic “fluid mechanics”.
5. Kaci Mcmillin, Barret Honors Project contracted with PHY321 course in fall 2018. Project topic “3D rigid body motion”.
6. Dante Roush, Barret Honors Project contracted with PHY321 course in fall 2018. Project topic “Kinetics of rigid bodies in 3D”.
7. Travis Giam, Barret Honors Project contracted with PHY321 course in fall 2017. Project topic “Design a self-balanced mechanical device with foldable arms”. Successfully completed the project and demonstrated the designed device on Dec. 2017.
8. Andrew Boateng, Barret Honors Project contracted with PHY321 course in fall 2017. Project topic “Analyze daily things using physics concept: Why does the bicycle tip over?” Successfully completed the project and submitted the report on Dec. 2017.

c) Obama Scholars

Supervised two Obama scholars during Fall 2010 – Spring 2011, providing advice on general studies and resources at ASU. Later on, both students took my General Physics courses.

9. Lawrence Gary
10. Christian Acosta

d) Undergraduate Researchers

11. Andre Brewer, summer 2014, “phospherene”, literature review.
12. Kason Ashe, Spring-fall 2011, “graphene”, delivered 1 conference presentation.
13. Phivu Nguyen, fall 2011, “InAs Nanowires”, co-authored 1 conference presentation.
14. Waleed Alsadi, fall 2011, “fuel cells”, literature review.
15. Sarah Salava, summer-fall 2010, “ZnO surface”, literature review.
16. Joshua Hoyt, spring 2010, “crown esters”, literature review.
17. Alan Bradford, spring 2009, “Molecule visualization”, literature review.
18. Selina Velasquez, spring-fall 2009, spring 2010, “graphene nanoribbons”, published 1 peer-reviewed paper; co-authored 3 conference presentations (delivered 1) and 5 ASU exhibit; Received Undergraduate Research Award from Applied Science of Math at ASU.

a) Senior Engineering Students in their Capstone Project in the College of Technology and Innovation

I mentored the College of Technology and Innovation Engineering Capstone project “On Semiconductor” in Fall 2010. Supervised senior students were:

19. Thomas Ward
20. Patrick Eberts
21. Jameson Smith
22. Fadi Hafez

23. Chris Chakkaw
24. Jonathan Cabizo
25. Michael Chacon.

III. SERVICE ACTIVITIES

H. ASU SERVICE

H1. Unit Level (Science and Mathematics Faculty and Dept. of Applied Sciences and Mathematics)

1. Teaching Evaluator of Instructional Specialists within the unit. (Fall 2008 – present).
2. *Chair on the Search Committee for the Tenure Track Assistant Professor in Applied Chemistry (Fall 2016 – Spring 2017).
3. Member of the Search Committee for the Tenure Track Assistant Professor in ABS/PreVet (Fall 2014 – Spring 2015)
4. Chair of the Search Committee for the Physics Instructor (Summer 2014).
5. Chair of the Search Committee for the Physics Instructional Professional (Spring 2014).
6. Committee Member of Faculty Teaching Evaluation (Fall 2013 – Spring 2014).
7. Committee Member of Unit Sabbatical Review (Fall 2013)
8. Member of the Search Committee for Lab Manager (Spring 2013).
9. Member of the Committee of Curriculum and Instruction (Fall 2010-Spring 2012).
10. Member of the Committee of Awards (Fall 2012 - present).
11. Member of the Search Committee for Physics Instructional Professional (Summer 2012).
12. Member of the Search Committee for two Physics Instructional Professionals (Summer 2011).
13. Member of the Search Committee for Physics Coordinator (Fall 2010).
14. Member of the Search Committee for Physics Instructional Specialist (Spring 2009).

H2. College Level (Colleges of Letters & Sciences, Technology & Innovation)

15. Committee Member of the College Personnel Committee (Spring 2016 – Spring 2019)
16. Member of the Search Committee for the Dean of College of Letters and Sciences (Fall 2014 – Spring 2015)
17. Member of the Committee of Alternative Energy Curriculum (Fall 2011 and Spring 2012).

I. PROFESSIONAL SERVICE

I1. Book Editor

- “Nanowires – Recent Advances”, ISBN 978-953-51-0898-6, **Xihong Peng** (Editor), 2012 In Tech. <http://www.intechopen.com/books/nanowires-recent-advances/>

I2. Journal Editor

- Review Editor at *Frontiers* which is an open-access academic publisher and research network. *Frontiers* was launched in 2007 now has become one of the largest and fastest-growing open-access scholarly publishers. *Fall 2014 – present*

I3. Referee for the Following Journals: (review on average ~ 6 or 7 per year)

1. Nature Communications
2. Nano Letters
3. Nanoscale
4. Advanced Functional Materials
5. Nanotechnology
6. Applied Physics Letters
7. Journal of Applied Physics
8. New Journal of Physics
9. Journal of Physical Chemistry
10. Physical Chemistry Chemical Physics
11. International Journal of Hydrogen Energy
12. Journal of Physics: Condensed Matter
13. Journal of Physics D: Applied Physics
14. Physica B: Condensed Matter
15. Chemical Physics
16. Chemical Physics Letters
17. Surface Science
18. Nanoscale Research Letters
19. Materials Research Letters
20. Computational Materials Science
21. Semiconductor Science and Technology
22. Materials Science in Semiconductor Processing

I4. Reviewer for Funding Agencies:

- University of Wisconsin-Milwaukee Research Growth Initiative.
- National Science Foundation (Division of Material Research).
- Czech Science Foundation (for standard proposals).

I5. Reviewer for Books or Book Chapters

- “University Physics for the Physical and Life Sciences”, authored by Kesten and Tauck, Chapter 13 Waves, W. H. Freeman & Company, March 2012.

J. COMMUNITY SERVICE

- Delivered total of five workshop lectures to the 2nd Grade classroom at ASU Preparatory Academy Elementary School during in spring, 2018.

- Delivered a workshop lecture to the 1st and 2nd Grader Classroom at ASU Preparatory Academic Elementary School at Polytechnic campus. (Jan 20th. 2017).
- Delivered total of five workshop lectures to the 1st Grade classroom at ASU Preparatory Academy Elementary School during in spring, 2017.
- Delivered total of five workshop lectures to the kinder classroom at ASU Preparatory Academy Elementary School during in fall, 2015.
- Exhibited “Explore what’s in store” to 8th and 9th graders in Mesa Convention Center (January 19th, 2012).
- Invited to give a lecture for 1 & 2 graders at ASU Preparatory Academy - Polytechnic Elementary School (November 10th, 2010).