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EMPLOYMENT

- ❖ **Professor**, ASU at the Polytechnic campus, Mesa, AZ *July 2021 – present*
- Graduate Faculty**, Department of Physics, ASU, Tempe *October 2008 – present*
- Graduate Faculty**, Materials Sciences, ASU, Tempe *February 2012 – present*
- Graduate Faculty**, Systems Engineering, ASU, Polytechnic *August 2018 - present*
- ❖ **Associate Professor**, ASU at the Polytechnic campus, Mesa, AZ *May 2014 – July 2021*
- ❖ **Assistant Professor**, ASU at the Polytechnic campus, Mesa, AZ *August 2008 – May 2014*
- ❖ **Postdoctoral Researcher**, Rensselaer Polytechnic Institute, Troy, NY *Oct. 2007 – Aug. 2008*
- ❖ **Visiting Assistant Professor**, Skidmore College, NY *September 2007 – May 2008*
- ❖ **Research Consultant**, General Electric, Global Research, NY *May 2005 – December 2005*
- ❖ **Research Intern**, General Electric, Global Research Center, NY *May 2004 – August 2004*

EDUCATION

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

HONORSHIP

VEBLEO FELLOW on Materials Science, Engineering and Technology since May 2021

I. SCHOLARLY ACTIVITIES**A. PUBLICATIONS****A1. Peer-Reviewed Journal Papers**

My **advised students** are underlined and in bold, my advised visiting students/scholars are denoted using †, and the corresponding authors are denoted using *.

Under review

1. **Andrew Dopilka**, Amanda Childs, Alexander Ovchinnikov, Ran Zhou, Svilen Bobev, **Xihong Peng**, Candace K. Chan*, “Structural and Electrochemical Properties of Type VIII $\text{Ba}_8\text{Ga}_{16}\text{-}\delta\text{Sn}_{30+\delta}$ Clathrate ($\delta \approx 1$) during Lithiation”, *ACS Applied materials & Interfaces*.

2. S. Ahmad†, Abid Ullah, Tahir Nawaz, Afaf Ali Kazmi†, Saim Saher*, **Xihong Peng**, A.M. Kannan, "Synthesis of MnO₂ nanorods with enhanced Oxygen Reduction Reaction for Proton Exchange Membrane Fuel Cell", *International Journal of Hydrogen Energy*.

Published:

3. Ying Yang†, Guang Yang†, **Xihong Peng***, "New stable 2D and 3D GeC₂ crystal structures predicted by first-principles study", *Materials Today Communications* **28**, 102567 (2021).
4. Yunqi Li, Jing Li, Yanggang Wang, Xiran Chen, Mingtao Liu, Zhong Zheng, **Xihong Peng**, "Carbon Corrosion Mechanism on Nitrogen-Doped Carbon Support - A Density Functional Theory Study", *International Journal of Hydrogen Energy* **46**, 13273-13282 (2021).
5. Qun Wei, Ying Yang†, Guang Yang†, **Xihong Peng***, "New stable two dimensional silicon carbide nanosheets", *Journal of Alloys and Compounds* **868**, 159201 (2021).
6. Andrew Dopilka, J. Mark Weller, Alexander Ovchinnikov, Amanda Childs, Svilen Bobev, **Xihong Peng**, Candace K. Chan*, "Structural Origin of Reversible Li Insertion in Guest-Free Type-II Silicon Clathrates", *Advanced Energy and Sustainability Research* **2**, 2000114, <https://doi.org/10.1002/aesr.202000114>, (2021)
7. Qun Wei, Ying Yang†, Alexander Gavrilov, **Xihong Peng***, "A new 2D auxetic CN₂ nanostructure with high energy density and mechanical strength", *Physical Chemistry Chemical Physics* **23**, 4353-4364 (2021).
8. Guang Yang†, Ying Yang†, **Xihong Peng***, "Systematic theoretical study of carbon nanotubes rolled from two dimensional tetrahex-carbon nanosheet", *Physical Review B* **102**, 235409 (2020).
9. Umesh Prasad, Jyoti Prakash, Xuan Shi, Sandeep K. Sharma, **Xihong Peng**, Arunachala M. Kannan*, "Role of alkali metals in BiVO₄ crystal structure for enhancing charge separation and diffusion length for photoelectrochemical water splitting", *ACS Applied Materials & Interfaces* **12**, 52808-52818 (2020).
10. Ying Yang†, Guang Yang†, **Xihong Peng***, "The Electronic Properties of Fluorine or Hydrogen Adsorbed Tetrahexcarbon: A First-Principle Study", *Applied Surface Science* **529**, 147150 (2020).
11. Guang Yang†, **Xihong Peng***, "Tunable magnetism by edge functionalization in zigzag green phosphorene nanoribbons", *Physics Letters A* **384**, 126672 (2020).
12. **Xihong Peng***, Qun Wei, Guang Yang†, "Enhanced carrier mobility in anisotropic tetrahex-carbon through strain engineering", *Carbon* **165**, 37-44 (2020).

13. Qun Wei, Guang Yang†, **Xihong Peng***, “Auxetic tetrahex carbon with ultrahigh strength and a direct band gap”, *Physical Review Applied* **13**, 034065 (2020).
14. **Chi Ma†**, Tianxing Ma, **Xihong Peng***, “Quantum confinement and edge effects on electronic properties of zigzag green phosphorene nanoribbons”, *Journal of Physics: Condensed Matter* **32**, 175301 (2020).
15. Jyoti Prakash, **Umesh Prasad**, **Xuan Shi**, **Xihong Peng**, Bruno Azeredo and Arunachala M. Kannan*, “Photoelectrochemical water splitting using lithium doped bismuth vanadate photoanode with near-complete bulk charge separation”, *Journal of Power Sources* **448**, 227418 (2020).
16. **Andrew Dopilka**, **Xihong Peng***, Candace K. Chan*, “Ab initio Investigation of Li and Na Migration in Guest Free Type I Clathrates”, *Journal of Physical Chemistry C* **123**, 22812-22822 (2019).
17. Qun Wei, Wen Tong, Bing Wei, Meiguang Zhang, **Xihong Peng***, “Six new silicon phases with direct band gaps”, *Physical Chemistry Chemical Physics* **21**, 19963-19968 (2019).
18. Qun Wei, Chenyang Zhao, Meiguang Zhang, Haiyan Yan, Bing Wei, **Xihong Peng***, “New stable structures of HeN₃ predicted using first-principles calculations”, *Journal of Alloys and Compounds* **800**, 505-511 (2019).
19. **Evan Garrison**, Candace K. Chan, **Xihong Peng***, “Size and strain effects on mechanical and electronic properties of green phosphorene nanoribbons”, *AIP Advance* **8**, 115124 (2018).
20. **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* **10** (44), 37981-37993 (2018).
21. **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).
22. 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).
23. 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).
24. **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).

25. **A. Arvay, J. 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).
26. **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).
27. 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).
28. **Xihong Peng***, Qun Wei†, “Chemical scissors cut phosphorene nanostructures”, *Materials Research Express* **1**, 045041 (2014).
29. **Xihong Peng***, **Andrew Copple**, Qun Wei†, “Edge effects on the electronic properties of phosphorene nanoribbons”, *Journal of Applied Physics* **116**, 144301 (2014).
30. **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).
31. Qun Wei†, **Xihong Peng***, “Superior mechanical flexibility of phosphorene and few-layer black phosphorus”, *Applied Physics Letters* **104**, 251915 (2014).
32. 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).
33. 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).
34. 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).
35. **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).
36. **A. Arvay, J. 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).

37. 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).
38. **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).
39. **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).
40. 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).
41. **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).
42. **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).
43. **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).
44. **X.-H. Peng***, **S. Velasquez**, “Strain modulated band gap of edge passivated armchair graphene nanoribbons”, *Applied Physics Letters* **98**, 023112 (2011).
45. **X.-H. Peng***, **P. Logan**, “Electronic properties of strained Si/Ge core-shell nanowires” *Applied Physics Letters* **96**, 143119 (2010).
46. 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).
47. **P. Logan**, **X.-H. Peng***, “Strain-modulated electronic properties of Ge nanowires: a first-principles study”, *Physical Review B* **80**, 115322 (2009).
48. **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).

49. 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).
50. 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).
51. **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).
52. **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).
53. **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).
54. K. Iyakutti*, A. Bodapati, **X.-H. Peng**, P. Koblinski, 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).
55. **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).
56. 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).
57. M. Zhan*, Z.-G. Zheng, G. Hu, **X.-H. Peng**, “Nonlocal chaotic phase synchronization”, *Physical Review E* **62**, 3552 (2000).

A2. 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), 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.

B. CONFERENCE ABSTRACT, PRESENTATIONS AND EXHIBITS

B1. Conference Abstract and 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***, “Material research using quantum mechanics computational methods, in application to low dimensional nanostructures and Li-ion batteries”, “International Conference on Condensed Matter and Device Physics (ICCMDP-2021), Gandhinagar, India, September 9th – 11th, 2021. (Invited Oral presentation)
2. **X.-H. Peng***, **A. Dopilka**, C. K. Chan, “Structural Origin of Reversible Li Insertion in Guest-Free, Type-II Silicon Clathrates for Applications as Li-ion Battery Anodes”, American Association for Advances in Functional Materials Conference at University of California, Los Angeles, August 18th -20th, 2021. (Invited Oral presentation)
3. **X.-H. Peng***, **A. Dopilka**, C. K. Chan, “Li and Na migration in guest-free, type I clathrates evaluated via *ab initio* methods”, American Physical Society (APS), 2020 March international meeting (Virtual online presentation, March 4th, 2020). <http://meetings.aps.org/Meeting/MAR20/Session/L21.12>
4. **C. Ma**†*, T. Ma, **X.-H. Peng**, “Quantum confinement and edge effects in zigzag green phosphorene nanoribbons”, American Physical Society (APS), 2020 March international meeting (Virtual online presentation, March 6th, 2020). <http://meetings.aps.org/Meeting/MAR20/Session/X65.9>
5. **X.-H. Peng***, **A. Dopilka**, C. K. Chan, “Lithiation of Si/Ge clathrates as anodes in Li-ion batteries”, The 10th International Symposium on Clusters and Nano-Structures (ISCAN), Richmond, VA (Poster presentation, November 6th, 2019).
6. **[Invited speech] X.-H. Peng***, **A. Dopilka**, C. K. Chan, “Computational study of lithiation of Ba-doped Type I Si/Ge clathrates”, the 2019 International Collaborative Conference on Materials Research (CCMR), Seoul, South Korea, June 03-07, 2019. (Oral presentation, June 6th, 2019).
7. **[Invited speech] X.-H. Peng***, **A. Dopilka**, C. K. Chan, “Computational study of lithiation of Si/Ge clathrates, towards application in high energy density Li-ion batteries”, the 4th

- International Conference on Energy Materials and Application, Beijing, China, May 11-13, 2019. (Oral presentation, May 13th, 2019).
8. **G. Yang**†, **E. Garrison**, T. Ma, **X.-H. Peng***, “Size and Strain Effects on Mechanical and Electronic Properties of 2D Green Phosphorene Monolayer and Nanoribbons”, Materials Research Society (MRS), 2019 spring international meeting & exhibit, Phoenix, AZ (Poster presentation, April 24th, 2019).
 9. **A. Dopilka***, R. Zhao, J. Weller, S. Bobev, **X.-H. Peng**, C. K. Chan, “Intermetallic clathrates as insertion anodes for Li-ion batteries”, Materials Research Society (MRS), 2019 spring international meeting & exhibit, Phoenix, AZ (Poster presentation, April 24th, 2019).
 10. **X.-H. Peng***, **A. Dopilka**, Q. Wei†, C. K. Chan, “Computational Study of Lithiation of Ba-Doped Type I Si/Ge Clathrates”, Materials Research Society (MRS), 2019 spring international meeting & exhibit, Phoenix, AZ (Oral presentation, April 26th, 2019).
 11. **G. Yang**†, T. Ma, **X.-H. Peng***, “Mechanical and electronic properties of 2D green phosphorene, a first-principles study”, American Physical Society (APS), 2019 March international meeting, Boston, MA (Poster presentation, March 7th, 2019).
<http://meetings.aps.org/Meeting/MAR19/Session/T70.288>
 12. **X.-H. Peng***, **A. Dopilka**, Q. Wei†, C. K. Chan, “First-Principles Study of Lithiation of Type I Ba-Doped Silicon and Germanium Clathrates”, American Physical Society (APS), 2019 March international meeting, Boston, MA (Oral presentation, March 4th, 2019).
<http://meetings.aps.org/Meeting/MAR19/Session/F47.7>
 13. **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).
<https://meetings.aps.org/Meeting/MAR16/Session/G1.44>
 14. **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).
<https://meetings.aps.org/Meeting/MAR15/Session/F17.13>
 15. **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).
<http://meetings.aps.org/Meeting/MAR14/Session/B50.8>
 16. **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).
<http://meetings.aps.org/Meeting/MAR13/Event/182800>
 17. **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).
<http://meetings.aps.org/Meeting/4CF12/Session/H4.4>

18. **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).
<http://meetings.aps.org/Meeting/4CF12/Session/E4.1>
19. **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).
<https://meetings.aps.org/Meeting/MAR12/Session/Q7.2>
20. **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).
21. **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).
<http://meetings.aps.org/Meeting/4CF11/Event/157591>
22. **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).
<https://ui.adsabs.harvard.edu/abs/2011APS..4CF.F1003N/abstract>
23. **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).
<http://meetings.aps.org/Meeting/4CF11/Event/157593>
24. **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).
<http://meetings.aps.org/Meeting/MAR11/Session/V11.1>
25. **P. Logan***, **X.-H. Peng**, “Electronic properties of strained Si [111] nanowires”, APS, 2010 March international meeting, Portland, OR (Poster presentation, March 15th, 2010).
<http://meetings.aps.org/Meeting/MAR10/Session/C1.105>
26. **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*”).
<http://meetings.aps.org/Meeting/4CF09/Session/D1.38>
27. **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).

<http://meetings.aps.org/Meeting/4CF09/Session/D1.37>

28. **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).
<http://meetings.aps.org/Meeting/MAR09/Session/J36.2>
29. **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).
30. **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).
31. **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).
32. **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).

B2. ASU Presentations and Exhibits

1. **Alexander (Sasha) Gavrillov, X.-H. Peng**, “Analyzing Mechanical Properties of Clathrates: The Quest for a Higher Energy Capacity Battery” at the Research Showcase, the College of Integrative Sciences and Arts (Poster presentation, November 28th, 2018).
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 Showcase (Poster presentation, April 25th, 2012).
3. **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).
4. **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).
5. **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).

6. **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).
7. **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. COLLOQUIUM AND SEMINAR TALKS

1. **(Invited Keynote Talk for Fellow of Vebleo)** “Material Research Using Quantum Mechanics Computational Methods”, Webinar on Material Science, Engineering and Technology, Vebleo, May 21st, 2021.
2. **(Invited)** “Material research using first-principles computational methods for applications in nanoelectronics and Li-ion batteries”, Nonlinear Science Theory and Intersection Seminar-Research on Extensive Synchronization of Complex Networks and Dynamic Stability of Smart Grid, School of Electrical and Electronic Engineering, Huazhong University of Science and Technology, December 5th, 2020.
3. “Material research using quantum mechanics computational method”, Science and Mathematics Seminar, College of Integrative Sciences and Arts, Arizona State University, September 9th, 2020.
4. **(Invited)** “Computational Research of materials for nanoscale semiconductors and Li-ion battery application”, Department of Physics, Virginia Commonwealth University, Richmond, VA, November 1st, 2019.
5. **(Invited)** “First principles density-functional theory calculations, projects overview”, Department of Electronic Engineering, Xi’an University of Technology, May 31st, 2019.
6. **(Invited)** “Computational materials research for applications in nano-semiconductors and Li-ion batteries”, School of Physics and Optoelectronic Engineering, Xidian University, May 31st, 2019.
7. **(Invited)** “First principles computational methods overview and tutorial on the VASP code”, School of Chemistry and Chemical Engineering, Hunan University, May 29th, 2019.
8. **(Invited)** “Computational materials research for applications in nano-semiconductors and Li-ion batteries”, School of Precision Instrument and Opto-Electronics Engineering, Tianjin University, May 21st, 2019.
9. **(Invited)** “Computational materials research for applications in nano-semiconductors and Li-ion batteries”, College of Engineering, Peking University, May 20th, 2019.
10. **(Invited)** “Materials research for applications in nano-electronics and renewable energies using computational methods”, Physics Department, Beijing Normal University, May 16th, 2019.

11. **(Invited)** “Materials research for applications in nano-electronics and renewable energies using first-principles computation”, Physics Department, Jiangnan University, Wuhan, China, May 4th, 2018.
12. “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.
13. **(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.
14. **(Invited)** “Frontier research of material sciences from the aspect of computational physics and chemistry”, Chemistry Department, Hunan University, Changsha, China, May 28th, 2015.
15. **(Invited)** “Computational materials research and applications in nano-electronics and renewable energies”, Chemistry Department, Hunan University, Changsha, China, June 9th, 2014.
16. “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.
17. **(Invited)** “Strain engineered electronic properties in semiconductor nanostructures”, Physics Department, Washington University in St. Louis, St. Louis, MO, February 25th, 2013.
18. **(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.
19. **(Invited)** “Energy gaps and quantum carriers in strained nanostructures”, Department of Physics, Applied Physics, and Astronomy, Rensselaer Polytechnic Institute, Troy, NY, February 20th, 2013.
20. **(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.
21. **(Invited)** “Predictive modeling for nanoscale system using first-principles calculations”, Beijing Computational Science Research Center, Beijing, China, May 24th, 2012.
22. “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.

23. **(Invited)** “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.
24. “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.
25. **(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.
26. **(Invited)** “Predictive modeling for nanoscale materials using first principles calculation”, Department of Physics, Arizona State University, Tempe, AZ, November 10th, 2008.
27. “Tunable luminescence from silicon quantum dots”, Department of Physics, University of Massachusetts, Dartmouth, MA, March 27th, 2008.
28. “Tunable luminescence from silicon quantum dots”, Department of Physics, University of Wisconsin-Eau Claire, Eau Claire, WI, March 11th, 2008.
29. “Tunable luminescence from silicon quantum dots”, Department of Physics, Westminster College, Fulton, MO, February 6th, 2008.
30. “Tunable luminescence from silicon quantum dots”, Department of Physics, Skidmore College, Saratoga Springs, NY, April 5th, 2007.
31. “Silicon quantum dots”, Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, Troy, NY, July 19th, 2006.

D. OTHER PROFESSIONAL/SCHOLARLY ACTIVITIES

1. **Invited Visiting Professor** in Department of Chemical Engineering, Hunan University, China, May 27 – 29, 2019, trained Ph.D. and master students to use quantum mechanical computation code VASP.
2. **Invited Visiting Professor** in Department of Physics, Beijing Normal University, China, May 10 – May 24, 2019. Worked on a collaborative projects and trained two Ph.D. students Chi Ma and Huijia Dai in the research group of Prof. T. Ma.
3. **Invited Visiting Professor** in Department of Physics, Jiangnan University, Wuhan, China, April 27 – May 5, 2018. Worked on a collaborative training program to graduate students with Profs. X.-L. Zhu and Y. Tian.
4. **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.

5. **Invited Visiting Professor** in Beijing Computational Science Research Center, China, May 20th – 27th, 2012, worked on a collaborative project on magnetic properties of graphene with Prof. T.-X. Ma.
6. **Invited Visiting Professor** in Department of Physics, Applied Physics and Astronomy, Rensselaer Polytechnic Institute, Troy, NY, USA, June 14th – 27th, 2009, worked on a project on strained graphene sheets in collaboration with Prof. S.K. Nayak.
7. **Invited Visiting Professor** in Department of Mechanical Engineering, University of Houston, Houston, TX, USA, May 19th – 25th, 2009, 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

E. TEACHING

Courses Taught at ASU, PHY121, 321, 495, 444, 499, 252, 111, 112, etc.

F. MENTORING

G1. Graduate Students

- 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 Master Degree of Science in Physics in Dec. 2013.
- 3) Master student Nathaniel Ralston (ASU, Tempe, Physics Department) on the projects of "III-V nanowires", and received the Master Degree of Science in Physics in May 2012.
- 4) 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 in Physics in May 2012.

- 5) Ph.D. student Andrew Dopilka (ASU, Tempe, Material Science) on the project of “Si/Ge/Sn clathrates as battery anode materials”, fall 2017- summer 2021, received the Ph.D. in July 2021.
- 6) Ph.D. student Xuan Shi (ASU, Polytechnic, Systems Engineering Program) on the project of “Pt/Pt Alloy and Manganese Dioxides Based Oxygen Reduction Reaction Catalysts for Low-Temperature Fuel Cells”, and received the Ph.D. in Engineering in Aug. 2019.
- 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 Master Degree of Science in Technology in December 2011.
- 8) Ph.D. student Grigoria Athanasaki (ASU, Poly, Systems Engineering) on the thesis titled “Design and Development of Gas Diffusion layers for Proton Exchange Membrane Fuel Cells at various Relative Humidity Conditions”, received Ph.D. in Engineering in May 2021.
- 9) Master student Jie Liu (Beijing Normal University (BNU), China, Physics Department) on the project of “First principles study of low dimensional structures of Ag_2Te ”, MS degree in Physics in June 2019.
- 10) Master student Lin Xu (BNU, Physics Department) on the project of “Metal-insulator phase transition and boundary magnetic properties of electron-correlation systems”, MS degree in Physics in June 2019.
- 11) Master student Juan Zhang (BNU, Physics Department) on the project of “Study the scalability and periodicity of Anderson model on honeycomb lattice”, MS degree in Physics in June 2019.
- 12) Master student Mathan Moorthy (ASU, Polytechnic, Engineering Department) on the project of “fuel cells”, MS degree in Technology in May 2015.
- 13) 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.
- 14) 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.
- 15) 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.

- 16) 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.
- 17) 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.
- 18) 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.
- 19) 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.
- 20) 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.
- 21) 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.
- 22) 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.
- 23) 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.
- 24) 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.
- 25) 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.
- 26) 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.

27) 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.

28) 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.

G2. 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 Honor's thesis**

- 1) Matthew Jones. Served as a Co-advisor of Matthew's honor's 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 Honor's projects**

- 1) Kristian Dolghier, Barret Honors Project contracted with PHY444 courses in spring 2021. Project topic "tetrahexa-SiC nanoribbons".
- 2) Reid Merrell, Barret Honors Project contracted with PHY121 course in spring 2021. Project topic "kinetic sculptures".
- 3) Zachary Norris, Barret Honors Project contracted with PHY121 course in spring 2021. Project topic "fluid mechanics".
- 4) Whitney Foster, Barret Honors Project contracted with PHY321 course in fall 2020. Project topic "Temperature and its effect on paintball trajectory".
- 5) Nathan Paul Saylor, Barret Honors Project contracted with PHY321 course in fall 2019. Project topic "trajectory motion of rockets".
- 6) Nathan Steven Fonseca, Barret Honors Project contracted with PHY121 course in fall 2019. Project topic "fluid mechanics".
- 7) Jaesang Hwang, Barret Honors Project contracted with PHY121 course in fall 2019. Project topic "fluid mechanics".
- 8) Bella Sebastian Recato, Barret Honors Project contracted with PHY121 course in fall 2019. Project topic "fluid mechanics".

- 9) Isabelle Maureen Thalman, Barret Honors Project contracted with PHY121 course in fall 2019. Project topic “fluid mechanics”.
- 10) Alexander Gavrilov, Barret Honors Project contracted with PHY121 course in fall 2018. Project topic “mechanical properties of Si/Ge clathrates”.
- 11) Jacob Tanaka, Barret Honors Project contracted with PHY121 course in fall 2018. Project topic “fluid mechanics”.
- 12) Kaci Mcmillin, Barret Honors Project contracted with PHY321 course in fall 2018. Project topic “3D motion of rigid body”.
- 13) Dante Roush, Barret Honors Project contracted with PHY321 course in fall 2018. Project topic “kinetics of rigid body in 3D”.
- 14) 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.
- 15) 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) Undergraduate Researchers

- 16) Kristian Dolghier, spring 2021, “nanoribbons of tetrahex silicon carbides”.
- 17) Elliott Alletto, spring 2021, “fundamentals of electronic structure calculations”.
- 18) Zhennan Shen, spring 2021, “fundamentals of quantum chemistry simulations”.
- 19) Kristian Dolghier, fall 2020, “fundamentals of density-functional theory calculations”.
- 20) Alexander Gavrilov, spring 2020, “Open framework clathrates”.
- 21) Alexander Gavrilov, spring 2019, “Si clathrate for Li-ion battery application”.
- 22) Andre Brewer, summer 2014, “phosphorene”, literature review.
- 23) Kason Ashe, spring-fall 2011, “graphene”, delivered 1 conference presentation.
- 24) Phivu Nguyen, fall 2011, “InAs Nanowires”, co-authored 1 conference presentation.
- 25) Waleed Alsadi, fall 2011, “fuel cells”, literature review.
- 26) Sarah Salava, summer-fall 2010, “ZnO surface”, literature review.
- 27) Joshua Hoyt, spring 2010, “crown esters”, literature review.
- 28) Alan Bradford, spring 2009, “Molecule visualization”, literature review.
- 29) 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.

d) Obama Scholars

Supervised Obama scholars by providing advice on general studies and resources at ASU. Later on, both students took my General Physics courses.

- 30) Lawrence Gary, fall 2010-spring 2011

31) Christian Acosta, fall 2010-spring 2011

e) Senior Engineering Students in the Capstone Project

I mentored the Engineering Capstone project “On Semiconductor” in fall 2010 and supervised the following senior students:

- 32) Thomas Ward, fall 2010
- 33) Patrick Eberts, fall 2010
- 34) Jameson Smith, fall 2010
- 35) Fadi Hafez, fall 2010
- 36) Chris Chakkaw, fall 2010
- 37) Jonathan Cabizo, fall 2010
- 38) Michael Chacon, fall 2010

G3. International Visiting Students/Scholars

a) As a faculty mentor for international visiting students/scholars

- 1) Ying Yang, visiting Scholar from Xi’an University of Technology, Research topic “electronic properties of silicon carbide”. Oct. 2019 – Oct. 2020.
- 2) Guang Yang, visiting Scholar from Hebei University of Science and Technology, Research topic “magnetism by edge functionalization in phosphorene nanoribbons”. Aug. 2019 – Aug. 2020.
- 3) Chi Ma, visiting Ph.D. student from Beijing Normal University, Research topic “zigzag green phosphorene nanoribbons”. Jul. 2019 – Nov. 2019.
- 4) Guang Yang, visiting Ph.D. student from Beijing Normal University, Research topic “green phosphorene”. Jul. 2017 – Dec. 2017.
- 5) Tianxing Ma, visiting Scholar from Beijing Normal University, Research topic “magnetism in graphene nanostructure”. Sept. 2012 & Mar. 2016.
- 6) Qun Wei, visiting Scholar from Xidian University, Research topic “two dimensional black phosphorene”. May 2013 - May 2014.

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

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

G4. High school Students

- 1) Spencer Austin, high school senior at BASIS Chandler, Senior Research Project to investigate the application of quantum computing to the calculation of God's number—the maximum number of moves required to solve any permutation of a Rubik's cube.

III. SERVICE ACTIVITIES**G. ASU SERVICE****H1. Unit Level (Sciences and Mathematics)**

1. *Chair on the Search Committee for the Lecturer Position in Applied Physics (fall 2020 – spring 2021).
2. Teaching Evaluator of other personnel within the unit, once or twice each academic year (fall 2008 – present).
3. Member in the Search Committee for the Lecturer Position in Applied Physics (fall 2019 – spring 2020).
4. *Chair on the Search Committee for the Tenure Track Assistant Professor Position in Applied Chemistry (fall 2016 – spring 2017).
5. *Chair on the Search Committee for the Physics Instructor Position (finished candidate screening and paperwork, skipped onsite interviews due to travel) (summer 2015).
6. Member in the Search Committee for the Position of Tenure Track Assistant Professor in Applied Biological Science/PreVet (fall 2014 – spring 2015).
7. *Chair on the Search Committee for the Physics Instructor Position (summer 2014).
8. *Chair on the Search Committee for the Position of Physics Instructional Professional (Spring 2014).
9. Member in the Faculty Teaching Evaluation Committee (fall 2013 – spring 2014).
10. Member in the Unit Sabbatical Review Committee (fall 2013).
11. Member in the Search Committee for the Lab Manager Position (spring 2013).
12. Member in the Curriculum and Instruction Committee (fall 2010-Spring 2012).
13. Member in the Awards Committee (fall 2012 – fall 2013).
14. Member in the Search Committee for the Position of Physics Instructional Professional (summer 2012).
15. Member in the Search Committee for two Positions of Physics Instructional Professionals (summer 2011).
16. Member in the Search Committee for the Physics Coordinator Position (fall 2010).
17. Member in the Search Committee for the Position of Physics Instructional Specialist (spring 2009).

H2. College Level (College of Integrative Sciences and Arts (CISA), Colleges of Letters & Sciences, Technology & Innovation)

1. Member in the College Tenure and Tenure-track Personnel Committee of CISA (fall 2019 – spring 2022).
2. Member of the College Tenure and Tenure-track Personnel Committee of CISA (fall 2016 – spring 2019).
3. Member in the Search Committee for the Dean’s Position of College of Letters and Sciences (fall 2014 – spring 2015).
4. Member in the Alternative Energy Curriculum Committee (fall 2011 and spring 2012).

H3. University Level (ASU)

1. Member in the University Senate, the Committee on Academic Freedom and Tenure (2020-2023).
2. Member in the University Research Computing Governance Board (7/1/2020-6/30/2021).
<https://cores.research.asu.edu/research-facilities-oversight-and-governance>
3. Member in the ASU Graduate College Interdisciplinary Enrichment Fellowship Review Committee (Academic Year 2019 -2020).
4. Member in the ASU Graduate College Achievement Rewards for College Scientists (ARCS) Fellowship Review Committee (AY 2018-2019, AY 2019-2020).
5. Member in the ASU Graduate College Completion Fellowship Review Committee (AY 2018-2019, AY 2019-2020).

H. PROFESSIONAL SERVICE

I1. Book Editor

1. “Nanowires – Recent Progress”, **Xihong Peng** (Editor), 2021 In Tech, in progress.
2. “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/Editorial Board

1. Special Issue Guest Editor, “Theoretical Condensed Matter Physics” in Applied Sciences (Impact Factor 2.217, Cite Score 2.52).
https://www.mdpi.com/journal/applsci/special_issues/theoretical_CMP *Dec. 2019 – present*
2. Editorial Board member as a Review Editor in Frontiers in Materials - Semiconducting Materials and Devices. *Dec. 2020 – present*
3. Editorial Board member of *Journal of Renewable and Green Energy*. *Spring 2019 – present*
4. Review Editor at *Frontiers in Nanotechnology (Nanotechnology for Energy Applications)*, Frontiers was launched in 2007 now has become one of the largest and fastest-growing open-access scholarly publishers. *Fall 2014 – present*

5. Editorial board member of *ScienceJet (Science Letters Journal)* which is an international, multi-disciplinary, peer reviewed, open access journal (Materials Sciences Section, Electronic materials sub-category). *Fall 2012 – Spring 2017*

I3. Referee for the Scientific Journals:

(For more than 20 journals, review on average ~ 6 or 7 articles per year)

- Nature Communications
- Nano Letters
- Nanoscale
- Advanced Functional Materials
- Nanotechnology
- Applied Physics Letters
- Journal of Applied Physics
- New Journal of Physics
- Journal of Physical Chemistry
- Physical Chemistry Chemical Physics
- International Journal of Hydrogen Energy
- Journal of Physics: Condensed Matter
- Journal of Physics D: Applied Physics
- Physica B: Condensed Matter
- Chemical Physics
- Chemical Physics Letters
- Surface Science
- Nanoscale Research Letters
- Materials Research Letters
- Computational Materials Science
- Semiconductor Science and Technology
- Materials Science in Semiconductor Processing

I4. Conference Organizer and Program Chair

1. A member in the International Organizing Committee, the international conference on Condensed Matter and Device Physics to be held in September 2021 in Gandhinagar, India.
2. A member of the Advisory/Organizing Committee, the international conference Advances in Functional Materials to be held in August 2021 at University of California, Los Angeles, USA.
3. Technical committee member, the International Conference on Energy materials and Applications, 2019.

4. Program session chair, the International Conference on Energy materials and Applications, 2019.

I5. Reviewer for the Funding Agencies:

1. National Science Foundation (Division of Materials Research), online reviewer, December 2020.
2. University of Wisconsin-Milwaukee Research Growth Initiative, online reviewer, 2014-2019.
3. The Netherlands e-Science Center and the Netherlands Organization for Scientific Research (NWO, the Dutch Research Council), July 2018.
4. National Science Foundation (Division of Materials Research), online reviewer, April 2013.
5. Czech Science Foundation (for standard proposals), online reviewer, October 2012.

I6. Reviewer for Books or Book Chapters

1. As a textbook chapter reviewer, "University Physics for the Physical and Life Sciences", authored by Kesten and Tauck, Chapter 13 Waves, W. H. Freeman & Company, March 2012.

I7. Reviewer for Other External Programs

1. As a program reviewer for the AP Physics curriculum, the College Board's Advanced Placement, Southern Regional Office, fall 2017.
2. As an external reviewer for the faculty promotion, MCPHS University, fall 2016.

I8. Invited Speakers on Forums and Salons

1. Invited Speaker in the Salon of Young Investigator Career Development, School of Physics and Optoelectronic Engineering, Xidian University, May 31, 2019.
2. Invited Speaker in the Project Review of Graduate Students Research of Prof. Yunqi Li, Department of Automotive Engineering, Advanced Vehicle Research Center, Beihang University, May 24, 2019.
3. Invited Speaker in the Salon of Undergraduate Career Planning and Development, Physics Department, Beijing Normal University, May 23, 2019.
4. Invited Speaker in the Forum of Physics Majored Students Career Planning, Physics Department, Jiangnan University, May 4, 2018.
5. Invited Speaker in the Forum of Master and Ph.D. Graduate Students Career Development, School of Chemistry and Chemical Engineering, Hunan University, May 28, 2015.

I. COMMUNITY SERVICE

1. Delivered a series of five workshop lectures to the 2nd grade classroom at ASU Preparatory Academy Elementary School during in spring, 2018.

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

PROFESSIONAL AFFILIATIONS

- ❖ Sigma Pi Sigma Honor Society, USA – Member since 2005.
- ❖ The American Physical Society, USA – Member since 2006.
- ❖ The American Chemical Society, USA – Member since 2012.
- ❖ The Material Science Society, USA – Member since 2018.