Qing Peng (Andrew)

Research Fellow, University of Michigan, Ann Arbor
Adjunct Professor, Wuhan University
2355 Bonisteel Blvd 1906 Cooley, Ann Arbor, MI 48109, U.S.A.
http://qpeng.org Email:qpeng@umich.edu Phone:+1(518)279-6669

Education

2005	Ph.D.	University of Connecticut, U.S.A.
2000	M.S.	State University of New York at Binghamton, U.S.A.
1998	B.S.	Peking University, China

Professional Positions

2016.10 –	Research Fellow, University of Michigan, Ann Arbor
2016.11 –	Visiting Research Scholar, Rensselaer Polytechnic Institute
2015.1 –	Adjunct Professor, Wuhan University, Wuhan, China
2012.9	Visiting Professor, Cardiff University, Cardiff, UK
2011.1-2016.9	Postdoctoral Research Associates, Rensselaer Polytechnic Institute
2010.1-2010.12	Postdoc Research Associates, Indiana Univ Purdue Univ Indianapolis
2009.11	Visiting Professor, Carnegie Institute of Washington
2007.1-2009.12	Postdoctoral Research Associates, California State University Northridge
2006.1-2006.12	Postdoctoral Research Associates, Carnegie Institute of Washington

Research Interests

- Multiscale modeling
- Nanomechanics
- Radiation damage
- Detonation of Energetic materials
- Thermoelectrics and energy harvesting
- Pyroelectrics,Ferroelectrics,Piezoelectrics
- Glasses and amorphous materials
- Polymer and biomaterials

Editorial Board

1. Scientific Reports (IF=5.578)
2. Graphene (IF=1.53)
3. Modeling and Numerical Simulation of Materials Science (IF=1.43)

Guest Editor

1. Crystals (IF=1.566)

Conference Chair

1. The 14th US National Congress on Computational Mechanics (USNCCM14) Symposium, Montreal, Canada,2017 (http://14.usnccm.org)
2. The 8th International Conference on Computational Methods (ICCM2017), Guilin,China,2017 (http://www.sci-en-tech.com/ICCM/index.php/iccm2017)
3. The 17th International Conference on Electronic Packaging Technology (ICEPT 2016) Wuhan, China, Aug 16-19 2016 (http://www.icept.org/en)
4. The 13th US National Congress on Computational Mechanics (USNCCM13) Symposium, San Diego, CA, USA, 2015
5. American Physical Society (APS) march meeting 2013: Session G11: Concurrent Multi-Length Scale Modeling, Baltimore, MD, 2013
6. 12th US National Congress on Computational Mechanics (USNCCM12) Symposium: Concurrent Multi-Length Scale Modeling: from Finite Elements to Atoms and Electrons, Raleigh, NC, USA, 2013
7. Asia Pacific Congress on Computational Mechanics (APCOM) 2013: Multiscale modelling and simulations: from quantum to continuum, Singapore, 2013

Grant Panels

1. The research programs funded by the Romanian Government through the National Council for Scientific Research, 2012
2. Romanian funding programs for research led by the National Council for Research and Development,2013
3. Executive Agency for Higher Education, Research, Development and Innovation Funding of Romanian,2014
4. Executive Agency for Higher Education, Research, Development and Innovation Funding of Romanian,2015
5. National Center of Science and Technology Evaluation, Ministry of Education and Science, Republic of Kazakhstan, 2015

Membership

- American Physical Society (APS)
- Materials Research Society (MRS)
- Optical Society of America (OSA)
- United States Association for Computational Mechanics (USACM)
- IEEE Components, Packaging, and Manufacturing Technology Society (CPMT)

Honors

- "Chutian Scholar", Hubei Province, China, 2017
- ♠ Honoree of the 44th Annual Service Recognition, Rensselaer Polytechnic Institute, 2016

Grants and Awards

1. Awards: "Chutian Scholar (Chutian Chair Professor)" Wuhan University, Hubei Province, China, 2017
2. Awards: "Shanxi Province Hundred Talents Program (Innovative Talent Team Project)", Institute of Coal Chemistry, Chinese Academy of Sciences, ShanXi, China, 2017
3. Nominee for "Blavatnik Award for Young Scientists", 2016
4. Granted participant of "Northwestern Polytechnical University Aoxiang Forum for Distinguished Young Scholars", Xian, China, 2016
5. The 6th most cited Computational Materials Science articles published since 2011
6. Granted participant of "Wuhan University International Forum for Interdisciplinary Sciences and Engineering", Wuhan, China, June 12, 2014
7. Granted participant of "Gordon Research Seminar" on Energetic Materials, June 14-15, Newry, ME, 2014
8. Nominee for "Blavatnik Award for Young Scientists", 2014
9. Granted participant of "East Lake International Forum on Frontiers of Science and Technology for Outstanding Overseas Young Scholars", Wuhan, China, Oct 06, 2012.
10. Sponsored "Outstanding Researcher" EB1b Lawful Permanent Residency by Rensselaer Polytechnic Institute, 2012.
11. Granted participant of SPIE Optics+Photonics conference,San Diego, CA, 2009.
12. Predoctoral Fellowship, University of Connecticut, 2001

Invited Referee for Journals (58)

1. Nature Communications
2. Physical Review Letters
3. Nano Letters
4. Nanoscale
5. Physical Review B
6. Physical Chemistry Chemical Physics
7. Journal of Applied Physics
8. The Journal of Physical Chemistry
9. RSC Advances
10. Physical Review A
11. Chemistry of Materials
12. Modelling and Simulation in Materials Science and Engineering
13. Journal of Materials Chemistry
14. Computational Materials Science
15. Journal of Elasticity

16. NANO
17. Journal of Physics :Condensed Matter
18. Journal of Physics D: Applied Physics
19. Journal of Electronic Materials
20. Physics E
21. Acta Materialia
22. Frontiers of Physics
23. IEEE Photonics Journal
24. Science of Advanced Materials
25. Superlattice and Microstructures
26. Materials Letters
27. Advances in Condensed Matter Physics
28. Carbon
29. Modern Physics Letters B
30. IEEE J. Quantum Electronics
31. European Physical Journal
32. Journal of Molecular Graphics and Modelling
33. World Journal of Engineering and Physical Sciences
34. PLOS One
35. Optical Materials
36. Chemistry Central Journal
37. International Journal of Thermophysics
38. Journal of Optics
39. Physica Status Solidi B: Basic Solid State Physics
40. Nanotechnology
41. Journal of Computational Chemistry
42. Optical Express
43. Surface Review and Letters
44. Physics Letters A
45. International Journal of Quantum Chemistry
46. The Journal of Experimental Nanoscience
47. Journal of Spacecraft and Rockets
48. International Journal of Recent advances in Mechanical Engineering (IJMECH)
49. Engineering Fracture Mechanics
50. BAOJ Nanotechnology

51. Journal of Materials Research
52. Journal of Vacuum Science and Technology A
53. Journal of Geophysics and Engineering
54. Chemical Physics Letters
55. Materials Characterization
56. Diamond and Related Materials
57. 2D Materials
58. Materials Horizons

TEACHING

Teaching Course

Instructor IEEE International Conference
Montpelier, France 2016
Multi-physics and multi-scale modeling in microelectronics manufacturing and application
Course outline (http://www.eurosime.org/courses.html)
(1) Models and simulates numerous processes in manufacturing, reliability and testing for the first time
(2) Provides the skills necessary for virtual prototyping and virtual reliability qualification and testing
(3) Demonstrates concurrent engineering and co-design approaches for advanced engineering design of microelectronic products
(4) Covers packaging and assembly for typical ICs, optoelectronics, MEMS, 2D/3D SiP, and nano interconnects
(5) Concurrent multiple-scale modeling covering continuum mechanics and first principles calculations
(6) Hybrid continuum mechanics, mesoscale, and atomistic modeling for mechanical behaviors.
(7) Information-passing temporal multiscale modeling of long-term system aging and failure.

Teaching Course

Adjunct Professor School of Power and Mechanical Engineering, WuHan University
WuHan, HuBei, China Summer, 2015
Micro-NanoMechanics and Molecular Dynamics Simulations
This course is for both graduate and undergraduate students. It consists of 20 lectures, 3 hours for each lecture. The lectures are:
(1) Introduction to micro/nano mechanics and modeling;
(2) Introduction to Linux and vim;
(3) Introduction to python and MPI programming;

(4) Introduction to Thermodynamics and Statistics Mechanics;
(5) Introduction to Molecular Dynamics modeling, the LAMMPS and vmd program package;
(6) System relaxation and geometry optimization in LAMMPS;
(7) Elastic constants;
(8) Tensile test modeling;
(9) Vacancies/voids;
(10) Nanoindentation;
(11) Fracture mechanics and fracture toughness modeling;
(12) Grain Boundary;
(13) Lattice crystal and dislocations;
(14) Shock waves and multiscale shock techniques;
(15) Equations of state;
(16) Radial distribution function and Central symmetrical parameter;
(17) Heat transport and thermal properties;
(18) Multiscale modeling and atomic/continuum scale coupling;
(19) Accelerated Molecular Dynamics;
(20) Chemical vapor deposition and the tfMC modeling.

Teaching Course
Teaching Assistant University of Connecticut
Storrs, CT, USA 2004 – 2005
Introduction to Astronomy
Instructed the laboratory work and observations for three semesters. Created and maintained course website, held weekly office hours and graded homework and quizzes, mid-term exams and finals.

Teaching Lab
Teaching Assistant University of Connecticut
Storrs, CT, USA 2002-2003
Instructed Advanced High School students of Optics/Lasers in Photonics lab (Prof. Chandra Roychoudhuri).

Students Mentor
Teaching Assistant University of Connecticut
Storrs, CT, USA 2002-2003
(1) Mentor of new teaching assistants to share teaching experiences in International Teaching Assistant Program (ITAP) of UCONN (summer, 2004). Supervised by Dr. Catherine Ross.
(2) Instructed Research Undergraduate (RU) students in research of material simulation (summer,2003).

Mentoring High School student Rensselaer Polytechnic Institute
Troy, NY, USA 2015 summer
(1) Aaron Liu : learning about Molecular Dynamics and using LAMMPS to perform Molecular Dynamics simulations; generated a large sheet of twisted-bilayer graphene suitable for

further experimentation; simulated twisted-bilayer graphene with both the Tersoff potentials and the AIREBO potential and the AIREBO potential provided better results for the components of the elastic constant not in the direction of the applied deformation; A few simulations were done at various temperatures (graduated in 2016, go on study in Michigan University).

Mentoring Undergraduate Rensselaer Polytechnic Institute
Troy, NY, USA 2011 – 2013
(1) Jared Crean : learning about Molecular Dynamics and using LAMMPS to perform Molecular Dynamics simulations; generated a large sheet of graphene suitable for further experimentation; simulated graphene with both the Tersoff potentials and the AIREBO potential and the AIREBO potential provided better results for the components of the elastic constant not in the direction of the applied deformation; A few simulations were done at various temperatures (graduated in 2013).
(2) Nomita Vazirani: learning about Molecular Dynamics and using LAMMPS to perform Molecular Dynamics simulations, especially the elastic constants of metals (Al, Cu, Au, Zr) at finite temperatures. (graduated in 2013)
(3) Francis Lam: MD simulations of graphene with polymers, especially PMMA; study the enhancement of the mechanical properties by the graphene or carbon nanotubes. (graduated in 2013)
(4) Chenguang Wen: learning about Molecular Dynamics and using LAMMPS to perform Molecular Dynamics simulations. (graduated in 2014)

Mentoring Graduate students Rensselaer Polytechnic Institute
Troy, NY, USA 2012 – 2016
(1) Chao Liang : learning first-principles calculations; study the mechanics of 2D materials, especially the non-linear elastic properties, high order elastic constants. (graduated in 2014)
(2) Liang Han: MD simulations of graphene, h-BN, graphyne for their mechanical and thermal properties. (graduated in 2014)
(3) Weihui Wang: Advanced mechanical properties of graphene including friction. (graduated in 2016).
(4) Andrew Gaul: DFT calculations of the thermoelectrics for their mechanical and thermomechanical properties with defect engineering.
(5) Xin Sun: learning MD and first-principles calculations; study the mechanical properties of 2D materials, especially the non-linear elastic properties and high order elastic constants.
(6) Jie Hou: Fitting EAM potentials from DFT calculations for radiation damage modeling of Fe-Al-Cr alloys.
(7) Binghui Deng: Modeling advanced mechanical properties of 2D materials using molecular dynamics simulations.

PROPOSAL WRITING

(*wrote more than 20 proposals.*)

Industry

EPCOS Inc. (TDK Group) 2015
NDA Approved
Title: "Studying Temperature Coefficient of Elastic Stiffness of Piezoelectric Materials (LiNbO3 based) through Ab Initio Methods"
PI: Suvranu De
Amount: $ 120k (1 year)
My role: *Preparation*
Note: can not be PI due to RPI's policy. It's **transferable** under contract and Non-Disclosure Agreement.

Federal Agencies

Defense Threat Reduction Agency,DOD 2012
Status Awarded
Title: "A Novel Multiscale QM-MD-SPH Computational Method for Heterogeneous Multi-component Reactive Systems"
PI: Gui-Rong Liu
Co-PI: Suvranu De
Amount: $ 750K (5 years)
My role: *Preparation*
Note: I'm in charge of the QM and MD parts. It's **transferable** *under contract*

PUBLICATION LIST

Publication overview
H-index: 20 (Google Scholar, ResearcherID, ResearchGate, ORCID)
Total papers: 73; (on July 4, 2017)

- **63 Peer-reviewed journal papers**
  - average impact factor: 3.462
  - Total citations: 1157
  - *first-* and *corresponding* authored: 42
- 6 Conference papers
- 4 Book chapters

Peer−reviewed Journal papers
Subtotal 63 (* denotes corresponding author)

[1] Q. Cao, J. Zhang, J. Du, H. Zhao, S. Liu and **Q. Peng** * , "Athermally Repair Nanoscale Defects in Optical Materials Using Femtosecond Laser", *Nanoscale*, (2017), **in press**, DOI: 10.1039/C7NR01599B [link] (IF=7.394)

[2] A. Gaul, **Q. Peng** * D.J. Singh, G. Ramanath, T. Borca-Tasciuc, "Pressure-induced insulator-to-metal transitions for enhancing thermoelectric power factor in bismuth telluride-based alloys", *Physical Chemistry Chemical Physics*, (2017), **19**, 12784–12793 [link] (IF=4.493)

[3] B. Deng, J. Hou, H. Zhu, S. Liu, L. Liu, Y. Shi, and **Q. Peng** * "The normal-auxeticity mechanical phase transition in graphene", *2D Materials*, (2017), **4**, 021020 [link] (IF=9.611)

[4] **Q. Peng** * X. Sun, H. Wang, Y. Yang, X. Wen, C. Huang, S. Liu, and S. De, "Theoretical prediction of a graphene-like structure of Indium Nitride: a promising excellent material for optoelectronics", *Applied Materials Today*, (2017), **7**, 169–178 [link]

[5] D. Cao, H. Li,. H. Ge, M. Ramos,**Q. Peng** A. Dearden, Z. Cao, Y. Yang, Y. Li, X. Wen , "Insight into Structure and Energy of Mo27SxOy clusters" *RSC Advances*, (2017), **7**, 9513-9520 [link] (IF=3.240)

[6] Y. Ouyang, Y. Xie, Z. Zhang, **Q. Peng** * and Y. Chen, "Very high thermoelectric figure of merit found in hybrid transition-metal-dichalcogenides", *Journal of Applied Physics*, (2016), **120**, 235109 [link] (IF=2.183)

[7] L. Zheng, X. Liu, Y. Meng, Y. Zhou, W. Guo, **Q. Peng** , Y. Yang, H. Jiao, Y. Li, and X. Wen, "How far away are the iron carbide clusters from the bulks?", *Physical Chemistry Chemical Physics*, (2016), **18**, 32944-32951 [link] (IF=4.493)

[8] S. Ye, Q. Cao, Q. Wang, T. Wang, and **Q. Peng** * , "A highly efficient, stable, durable, and recyclable filter fabricated by femtosecond laser drilling of a titanium foil for oil-water", *Scientific Reports*, (2016), **6**, 37591 [link] (IF=5.578)

[9] G.Y. Wang, G.R. Liu, **Q. Peng**, and S. De, "A SPH implementation with ignition and growth and afterburning models for aluminized explosives", *International Journal of Computational Methods*, (2017), **14**, 1750046 [link] (IF=1.123)

[10] Z. Zhang, Y. Xie, **Q. Peng**, Y. Chen, "Phonon transport in single-layer boron nanoribbons" *Nanotechnology*, (2016) **27**,445703, [link] (IF=3.821)

[11] Y. Meng, X. Liu, C. Huo, W. Guo, D. Cao, **Q. Peng**, A. Dearden, X. Gonze, Y. Yang, J. Wang, H. Jiao, Y. Li, and X. Wen, "When Density Functional Approximations Meet Iron Oxides" *Journal of Chemical Theory and Computation*, (2016) **12**(10),5132 - 5144 [link] (ACS Editors' Choice) (IF=5.301)

[12] **Q. Peng** * W. Ji, J. Lian, F. Gao, S. Peng, H. Huang, and S. De, "A first-principles study of the avalanche pressure of alpha zirconium" *RSC Advances*, (2016) **6**, 72551 - 72558 [link] (IF=3.840)

[13] X. Liu, S. Zhao, M. Yu, **Q. Peng**, C. Huo, Y. Yang, Y. Li, and X. Wen, "Mossbauer Spectroscopy of Iron Carbides: From Prediction to Experimental Confirmation" *Scientific Reports*, (2016), **6**, 26184 [link] (IF=5.578)

[14] Y. Ding, **Q. Peng**, L. Gan, R. Wu, X. Ou, Q. Zhang, and Z. Luo, "Stacking modes induced reactivity enhancement for twisted bilayer graphene" *Chemistry of Materials*, (2016) **28**, 1034–1039 [link] (IF=8.354)

[15] Z. Zhang, Y. Xie, **Q. Peng**, Y. Chen, "A theoretical prediction of super high-performance thermoelectric materials based on MoS2/WS2 nanoribbons" *Scientific Reports*, (2016) **6**, 21639 [link] (IF=5.578)

[16] W. Wang, **Q. Peng**, Y. Dai, Z. Qian, S. Liu, "Distinctive nanofriction of graphene coated copper foil", *Computational Materials Science*, (2016), **117**, 406–411 [link] (IF=2.131)

[17] W. Wang, **Q. Peng**, Y. Dai, Z. Qian, S. Liu, "Temperature dependence of Raman spectra of graphene on copper foil substrate", *Journal of Materials Science: Materials in Electronics*, (2016), **117**, 406–411 [link] (IF=1.569)

[18] Y. Dai, S. Li, H. Gao, W. Wang, Q. Sun, **Q. Peng**, C. Gui, Z. Qian, S. Liu, "Properties of AlN film grown on Si (111)", *Journal of Crystal Growth*, (2016), **435**, 76–83 [link] (IF=1.698)

[19] Y. Dai, S. Li, H. Gao, W. Wang, Q. Sun, **Q. Peng**, C. Gui, Z. Qian, S. Liu, "Stress evolution in AlN and GaN grown on Si (111): experiments and theoretical modeling", *Journal of Materials Science: Materials in Electronics*, (2016), **27**, 2004–2013 [link] (IF=1.569)

[20] Y. Dai, W. Wang, C. Gui, X. Wen, **Q. Peng**, S. Liu, "A first-principles study of the mechanical properties of AlN with Raman verification" *Computational Materials Science*, (2016), **112**, 342–346 [link] (IF=2.131)

[21] Z. Zhang, Y. Xie, **Q. Peng**, Y. Chen, "Thermal transport in MoS2/ Graphene hybrid nanosheets" *Nanotechnology*, (2015), **26**, 375402 [link] (IF=3.821)

[22] **Q. Peng** *, L. Han, J. Lian, X. Wen, S. Liu, Z. Chen, N. Koratkar, and S. De "Mechanical Degradation of Graphene by Epoxidation: Insight from First-principles Calculations" *Physical Chemistry Chemical Physics*, (2015), **17**, 19484–19490 [link] (IF=4.493)

[23] G. Wang, **Q. Peng** *, G.R. Liu, and S. De "Microscopic study of Equation of State of β-HMX using reactive molecular dynamics simulations" *RSC Advances*, (2015), **5**, 55892–55900 [link] (IF=3.840)

[24] **Q. Peng** *, Rahul, G. Wang, G.R. Liu, S. Grimme, and S. De, "Predicting Elastic Properties of β-HMX from First-principles calculations", *The Journal of Physical Chemistry B*, **119**, 5896–5903 (2015) [link] (IF=3.302)

[25] Z. Zhang, Y. Xie, **Q. Peng**, and Y. Chen, "Geometry, stability and thermal transport of hydrogenated graphene nanoquilts" *Solid State Communications*, **213**, 31–36, (2015) [link] (IF=1.897)

[26] **Q. Peng***, A. K. Dearden, X. Chen, C. Huang, X. Wen, and S. De, "Peculiar pressure effect on Poisson ratio of graphone as a strain damper", *Nanoscale*, **7**, 9975–9979, (2015). [link] (Communications) (IF=7.394)

[27] **Q. Peng*** , Z. Chen and S. De, "A density functional theory study of the mechanical properties of graphane with van der Waals corrections", *Mechanics of Advanced Materials and Structures*, **22**, 717–721, (2015), [link] (IF=0.773)

[28] **Q. Peng***, L. Han, X. Wen, S. Liu, Z. Chen, J. Lian, and S. De, "Mechanical properties and stabilities of g-ZnS monolayers", RSC Advances, (2015), **5**, 11240 - 11247 [link] (IF=3.840)

[29] **Q. Peng***, L. Han, X. Wen, S. Liu, Z. Chen, J. Lian, and S. De, "Mechanical properties and stabilities of alpha Boron monolayers", Physical Chemistry Chemical Physics, (2015), **17**(3), 2160 - 2168. [link] (IF=4.493)

[30] G.Y. Wang, G.R. Liu, **Q. Peng**, S. De, D.L. Feng, M.B. Liu, "A 3D smoothed particle hydrodynamics method with reactive flow modeling for the simulation of ANFO explosives", Propellants, Explosives, Pyrotechnics, (2015), **40**, 566–575 [link] (IF=1.604)

[31] **Q. Peng*** and S. De, "Elastic limit of silicane", *Nanoscale*, (2014), **6**, 12071–12079 [link] (IF=7.394)

[32] **Q. Peng*** , Rahul, G. Wang, G.R. Liu, and S. De, "Structures, Mechanical Properties, Equations of State, and Electronic Properties of beta-HMX under Hydrostatic Pressures: A DFT-D2 study", *Physical Chemistry Chemical Physics*, (2014), **16**, 19972-19983. [link] (IF=4.493)

[33] **Q. Peng***, W. Ji, J. Lian, X. Chen, H. Huang, F. Gao, and S. De, "Pressure effect on stabilities of self-Interstitials in HCP-Zirconium", *Scientific Reports*, **4**, 5735 (2014). [link] (IF=5.578)

[34] **Q. Peng***, A. Dearden, J. Crean, Y. Xu, S. Liu, C. Huang, X. Wen, and S. De, "New materials graphyne, graphdiyne, graphone, and graphane: review of properties, synthesis, and application in nanotechnology", *Nanotechnology, Science and Applications*, **7**, 1–29 (2014). [link] (Editor Invited Review) (IF=0.780)

[35] C. Huang, F. Libisch, **Q. Peng**, and E.A. Carter, "Time-dependent potential functional embedding theory", *The Journal of Chemical Physics*, **140**, 124113 (2014). [link] (IF=2.952)

[36] **Q. Peng*** and S. De, "Mechanical properties and instabilities of ordered graphene oxide C6O monolayers", *RSC Advances*, **3**, 24337–24344 (2013). [link] (IF=3.840)

[37] **Q. Peng*** and S. De, "Outstanding mechanical properties of monolayer MoS2 and its application in elastic energy storage", *Physical Chemistry Chemical Physics*, **15**, 19427–19437 (2013). [link] (IF=4.493)

[38] Y. Sun, **Q. Peng**, and G. Lu, "Quantum Mechanical Modeling of Hydrogen Assisted Cracking in Aluminum", *Physical Review B*, **88** 104109 (2013). [link] (IF=3.736)

[39] **Q. Peng*** , C. Liang, W. Ji and S. De, "Mechanical Properties of g-GaN: A First Principles Study", *Applied Physics A*, **113**, 483–490 (2013). [link] (IF=1.704)

[40] **Q. Peng*** , J. Crean, A. Dearden, C. Huang, X. Wen, S. P. A. Bordas, and S. De, "Defect engineering of 2D monatonic-layer materials", *Modern Physics Letters B*, **27**, 1330017 (2013). [link] (Editor Invited Review) (IF=0.746)

[41] **Q. Peng*** , X. Chen, W. Ji and S. De, "Chemically Tuning Mechanics of Graphene by BN", *Advanced Engineering Materials*, **15**, 718–727 (2013). [link] (IF=1.758)

[42] **Q. Peng*** , X. Wen and S. De, "Mechanical stabilities of silicene", *RCS Advances*, **3**, 13772–13781 (2013). [link] (IF=3.840)

[43] **Q. Peng*** , C. Liang, W. Ji and S. De, "A First-principles Study of the Mechanical Properties of g-GeC", *Mechanics of Materials*, **64**, 135–141 (2013). [link] (IF=2.329)

[44] **Q. Peng*** , X. Chen, S. Liu and S. De, "Mechanical Stabilities and Properties of Graphene-like Aluminum Nitride Predicted from First-principles Calculations", *RCS Advances*, **3**, 7083–7092 (2013). [link] (IF=3.840)

[45] **Q. Peng*** , W. Ji, H. Huang and S. De, "Axial Ratio Dependence of the Stability of Self-Interstitials in HCP Structures", *Journal of Nuclear Materials*, **437**, 293–296 (2013). [link] (IF=1.865)

[46] **Q. Peng*** , C. Liang, W. Ji and S. De, "A Theoretical Analysis of the Effect of the Hydrogenation of Graphene to Graphane on Its Mechanical Properties", *Physical Chemistry Chemical Physics*, **15**, 2003–2011 (2013). [link] (IF=4.493)

[47] **Q. Peng*** , W. Ji and S. De, "Strain Effect on Radiation Hardness: A First-Principles Study of the Hexagonal Boron Nitride Monolayer", *Nanoscale* **5**,695–703 (2013). [link] (IF=7.394)

[48] **Q. Peng*** , C. Liang, W. Ji and S. De, "A First Principles Investigation of the Mechanical Properties of g-ZnO: the Graphene-like Hexagonal Zinc Oxide Monolayer", *Computational Materials Science*, **68**, 320–324 (2013). [link] (IF=2.131)

[49] **Q. Peng*** , C. Liang, W. Ji, and S. De, "A First Principles Investigation of Mechanical Properties of g-TlN", *Modeling and Numerical Simulation of Material Science*, **2**, 76–84 (2012). [link] (IF=0.410)

[50] **Q. Peng*** , A. R. Zamiri, W. Ji, and S. De, "Elastic Properties of Hybrid Graphene/Boron Nitride Monolayer", *Acta Mechanica*, **223**, 2591–2596 (2012). [link] (IF=1.465)

[51] **Q. Peng*** , W. Ji, and S. De, "Mechanical Properties of Graphyne Monolayer: A First-Principles Study", *Physical Chemistry Chemical Physics*, **14**, 13385–13391 (2012). [link] (IF=4.493)

[52] **Q. Peng*** , W. Ji, H. Huang and S. De, "Stability of Self-interstitials in hcp-Zr", *Journal of Nuclear Materials*, **49**, 233–236, (2012) [link] (IF=1.865)

[53] **Q. Peng*** , W. Ji and S. De, "Mechanical Properties of the Hexagonal Boron Nitride Monolayer: ab initio Study". *Computational Materials Science*, **56**, 11 (2012). [link] *the 6th most cited Computational Materials Science paper since 2011* [link to report] (IF=2.131)

[54] **Q. Peng*** , and S. De, "Tunable Band Gaps of Mono-layer Hexagonal BNC Heterostructures", *Physica E: Low-dimensional Systems and Nanostructures*, **44**, 1662–1666 (2012). [link] (IF=2.000)

[55] **Q. Peng*** and R. E. Cohen, "Origin of Pyroelectricity in LiNbO3". *Physical Review B*, **83**, 220103(R) (2011). [link] (Rapid Communications) (IF=3.736)

[56] **Q. Peng*** and G. Lu, "A comparative study of fracture in Al: quantum mechanical vs. empirical atomistic description", *Journal of the Mechanics and Physics of Solids*, **59**, 775–786 (2011). [link] ("Featured Articles" in Advances In Engineering) (IF=3.598)

[57] Y. Zhao, C. Wang, **Q. Peng** and G. Lu, "Error Analysis and Applications of a General QM/MM Approach", *Computational Materials Science*, **50**, 714 (2010). [link] (IF=2.131)

[58] X. Zhang, **Q. Peng** and G. Lu, "Self-consistent embedding quantum mechanics/molecular mechanics method with applications to metals.", *Physical Review B*, **82**, 134120 (2010). [link] (IF=3.736)

[59] **Q. Peng***, X. Zhang, C. Huang, E. A. Carter and G. Lu, " Quantum Mechanical Study of Solid Solution Effects on Dislocation Nucleation During Nanoindentation", *Modelling and Simulation in Materials Science and Engineering*, **18**, 075003 (2010). [link] (IF=2.167)

[60] **Q. Peng***, X. Zhang and G. Lu, "Structure, mechanical and thermodynamic stability of vacancy clusters in Cu", *Modelling and Simulation in Materials Science and Engineering*, **18**, 055009 (2010). [link] (IF=2.167)

[61] **Q. Peng***, X. Zhang, and G. Lu, " Quantum mechanical simulations of nanoindentation of Al thin film", *Computational Materials Science*, **47**, 769 (2010) [link] (IF=2.131)

[62] **Q. Peng**, X. Zhang, L. Hung, E. A. Carter and G. Lu, "Quantum Simulation of Materials at Micron Scales and Beyond", *Physical Review B*, **78**, 054118 (2008). [link] (Editors' Suggestion) (IF=3.736)

[63] M. Utz, **Q. Peng** and M. Nandagopal, "Athermal simulation of plastic deformation in amorphous solids at constant pressure", *Journal of Polymer Science Part B: Polymer Physics*, **42**, 2057–2065 (2004). [link] (IF=3.803)

Conference Proceedings (full paper)

(Subtotal: 6)

[1] **Q. Peng***, G. Wang, G. R. Liu, and S. De, "Modeling the material strength and equations of state of beta-HMX from both first-principles calculations and molecular dynamics simulations", 19th Biennial Conference on Shock Compression of Condensed Matter (SCCM-2015), Location: Tampa, FL, USA, 2015

[2] G. Wang, G. R. Liu, **Q. Peng** and S. De, "A micro-macro coupling approach of MD-SPH method for reactive energetic materials", 19th Biennial Conference on Shock Compression of Condensed Matter (SCCM-2015), Location: Tampa, FL, USA, 2015 [online] [local PDF]

[3] **Q. Peng*** and S. De, "A first-principles investigation of the equation of states and molecular weak spots of β-cyclotetramethylene tetranitramine (HMX)", 15th International Detonation Symposium Location: San Francisco, CA, 2014 [link] [local PDF]

[4] **Q. Peng***, M. A. Barootkoob, C. Roychoudhuri, "What can we learn by differentiating between the physical processes behind interference and diffraction phenomena?", *Proceedings of SPIE*, **7421**, 74210B (2009). [link:DOI:10.1117/12.828572] [local PDF]

[5] G. Lu, **Q. Peng**, X. Zhang, L. Hung and E. A. Carter, *Oberwolfach Reports*, Volume 5, Issue 2, 1117 (2008) [link:DOI:10.4171/OWR/2008/21] [local PDF]

[6] C. Roychoudhuri, N. S. Prasad and **Q. Peng**, " Can the hypothesis 'photon interferes only with itself' be reconciled with superposition of light from multiple beams or sources? *Proceedings of SPIE*, **6664**, 66640S (2007). [link:DOI: 10.1117/12.734363] [local PDF]

Book Chapters

(Subtotal: 4)

[1] **Q. Peng**, "First-Principles Quantum Simulations", Chapter 1 in book "Nanoindentation in Materials Science", edited by Jiri Nemecek. (2012) InTechOpen, Australia. ISBN 980-953-307-282-6. [link:open access]

[2] **Q. Peng** * and S. De, "Mechanical stabilities and properties of graphene, and its modification by BN predicted from first-principles calculations", Chapter 5 in book "Graphene Science Handbook", Vol 4 "Mechanical and Chemical Properties", edited

by Mahmood Aliofkhazraei, Nasar Ali, William I. Milne, Cengiz S. Ozkan, Stanislaw Mitura, and Juana L. Gervasoni. (2016) CRC Press, Print ISBN: 978-1-4665-9123-3, eBook ISBN: 978-1-4665-9124-0, [local PDF]

[3] Lai Jiang, Zehao Yang, and **Q. Peng** *, "Mechanical Stabilities and Properties of Graphene-like Two-Dimentional III-Nitrides", in book "Computational and TheoreticalNanoscience of Two-Dimensional Materials", edited by Renqiang Zhu. (2016) Springer.

[4] **Q. Peng** *, X. Wen, S. De, "A review of the mechanical properties and structure instabilities of silicene" in book "Silicene: Structures, Properties and Functions", (2016) Nova Science.

PRESENTATIONS

Total 61

Plenary **Talks**

Subtotal 2

[1] "The normal-auxeticity mechanical phase transition and mechanochemistry in graphene", on World Chemistry Conference and Exhibition, Sep 04 - 06, 2017, Rome, Italy

[2] "Multiscale modeling in Computational Materials Science", on "7th International Advances in Applied Physics and Materials Science Congress" (APMAS2017) April 22, 2017 in Oludeniz, Fethiye, TURKEY.

Keynote **Talks**

Subtotal 1

[1] "Hydrogen Assisted Cracking in HCP-Zirconium: a Quasi-Continuum Density Functional Theory (QCDFT) Study", on 14th U.S. National Congress on Computational Mechanics July 17 - 20, 2017, Montreal, Canada

Invited *Conference* Talks

Subtotal 8

[1] "Quantum simulations of materials at large scale by QCDFT",Qing Peng, Oct 7, 2012. "East Lake International Forum on Frontiers of Science and Technology for Outstanding Overseas Young Scholars", Huazhong University of Science Technology, Wuhan, China.

[2] "What can we learn by differentiating between the physical processes behind interference and diffraction phenomena?", Qing Peng, Michael A. Barootkoob, Chandrasekhar Roychoudhuri, Aug 3, 2009, SPIE Meeting, San Diego, CA

[3] "An Accelerated Quasicontinuum-DFT (QCDFT) Method and its Application to Radiation Damage Modeling", Qing Peng and Suvranu De, 11th U.S. National Congress on Computational Mechanics. Jul 26, 2011, Minneapolis, Minnesota.

[4] "A Two-dimensional Jelly: Mechanical properties of graphyne",Qing Peng, Wei Ji and Suvranu De, Sept 25, 2012, 22nd International Workshop on Computational Mechanics of Materials (IWCMMXXII), Baltimore, MD

[5] "A real three-dimensional QCDFT model and its applications", Qing Peng and Suvranu De, 12th U.S. National Congress on Computational Mechanics. Jul 24, 2013, Raleigh, North Carolina.

[6] "A first-principles investigation of the crystal structure, elastic properties, and equation of states of
beta-cyclotetramethylene tetranitramine (HMX)", Qing Peng, June 14–15, 2014
bf Gordon Research Seminar on Energetic materials, Sunday River Resort in Newry, ME.

[7] "QCDFT concurrent multiscale modeling of hydrogen assisted cracking ",13th U.S. National Association for Computational Mechanics, Jul 26, 2015 San Diego, USA,

[8] "QCDFT concurrent multiscale modeling of hydrogen assisted cracking ", "Aoxiang Forum for Distinguished Young Scholars", Dec 20, 2016, Northwestern Polytechnical University, XiAn, China.

Conferences

(Subtotal 28)

[1] "Computer Simulation of The Localization of Plastic Shear Events in Molecular Glasses", Qing Peng, Marcel Utz, March 30, 2005, Materials Research Society (MRS) Spring Meeting, San Fransisco, CA

[2] "Novel Approach to Study of the Localization of Plastic Relaxation Events in Plastic Deformation of Amorphous Polymers", Qing Peng, Marcel Utz, March 24, 2005, American Physical Society (APS) March Meeting, Los Angeles, CA [htmlrefLinkhttp://meetings.aps.org/Meeting/MAR05/Event/24641]

[3] "First Principle Based Computation of Pyroelectricity in LiNbO3", Q. Peng, R. E. Cohen, March 18,2010, APS March Meeting, Portland, OR [htmlrefLinkhttp://meetings.aps.org/Meeting/MAR10/Event/122728]

[4] "Quantum Mechanical Simulations of Nanoindentation of Al Thin Film with Mg impurities", Qing Peng, Xu Zhang, Chen Huang, Emily A. Carter, Gang Lu, March 17,2010, APS March Meeting, Portland, OR [htmlrefLinkhttp://meetings.aps.org/Meeting/MAR10/Event/121616]

[5] "Functional Polar Materials by Design",R.E. Cohen, Q. Peng, and P. Ganesh, May 11 2010, 2010 U.S. Navy Workshop on Acoustic Transduction Materials and Devices, State College, Pennsylvania.

[6] "Computational Studies of the Reduction and Adsorption Mechanisms of Ethylene Carbonate on the Surface of Carbon Anodes of Lithium ion Batteries". Qing Peng, Zhiyao Duan and Guofeng Wang, Dec 3, 2010, MRS Fall 2010 Meeting, Boston, MA [htmlrefLinkhttp://www.mrs.org/f10-abstract-kk]

[7] "Origin of Pyroelectricity and the Electrocaloric Effect in LiNbO3", Q. Peng, P. Ganesh and R. E. Cohen, Jan 31 2011, Fundamental Physics of Ferroelectrics and Related Materials 2011, NIST, Gaithersburg, MD USA

[8] "A QCDFT Study of Hydrogen embrittlement at Crack Tip", Qing Peng, Mar 22, 2011, APS March Meeting, Dallas, TX. [htmlrefLinkhttp://meetings.aps.org/Meeting/MAR11/Event/139168]

[9] "The Temperature Dimension in First-principles Predictions of Properties of Piezoelectrics", R.E. Cohen, P. Ganesh, and Q. Peng, 2011 International Workshop on Acoustic Transduction Materials and Devices. May 12, 2011 The Penn Stater Conference Center Hotel, State College, Pennsylvania.

[10] "Electrocaloric Effect in LiNbO3 as functions of pressure and temperature",Ronald Cohen,Maimon Rose,Qing Peng,P. Ganesh, Energy Frontier Research Centers Summit and Forum 2011, May 25,2011, Washington,DC.

[11] "Time diffraction produced by a Talbot grating immersed in a dispersive medium",Qing Peng,Chandra Roychoudhuri, Suvranu De. Aug 24, 2011. SPIE Meeting, San Diego, CA.

[12] "Hydrogen Embrittlement in Zirconium: a Quasi-Continuum Density Functional Theory Study",Qing Peng, Feb 27, 2012. APS meeting, Boston, MA.

[13] "Golden Rule of Radiation Hardness: a Study of Strain Effect on Controlled Radiation Damage",Qing Peng, Mar 1st, 2012. APS meeting, Boston, MA.

[14] "A comparative study of fracture in Al: quantum mechanical vs. empirical atomistic description",Qing Peng, Gang Lu, Sept 24, 2012, 22nd International Workshop on Computational Mechanics of Materials (IWCMMXXII), Baltimore, MD

[15] "A Theoretical Analysis of the Effect of the Hydrogenation of Graphene to Graphane on Its Mechanical Properties",Qing Peng, Wei Ji and Suvranu De, Mar 19, 2013 APS March meeting, Baltimore, MD

[16] "Monovacancy in hcp-Zirconium",Qing Peng, Wei Ji, Hanchen Huang and Suvranu De, Mar 20, 2013 American Physical Society (APS) March meeting, Baltimore, MD

[17] "Outstanding mechanical properties of monolayer MoS_2 and its application in elastic energy storage", Qing Peng and Suvranu De, Mar 4, 2014 American Physical Society (APS) March meeting, Denver, Colorado.

[18] "Quantum mechanical modeling of hydrogen assisted cracking in aluminum", Qing Peng, Yi Sun, and Gang Lu, Mar 4, 2014 American Physical Society (APS) March meeting, Denver, Colorado.

[19] "Elastic limit of silicane", Qing Peng and Suvranu De, June 18 2014, The 17th U.S. National Congress on Theoretical and Applied Mechanics (USNCTAM), East Lansing, Michigan.

[20] "Crystal structure, elastic properties, and equation of states of
beta-HMX: A DFT-D2 study", Qing Peng, Jun 19, 2014
bf Gordon Research Conference on Energetic materials, Sunday River Resort in Newry, ME.

[21] "A first-principles investigation of the crystal structure, elastic properties, and equation of states of
beta-cyclotetramethylene tetranitramine (HMX)", Qing Peng and Suvranu De, July 13–18, 15th International Detonation Symposium (IDS), San Francisco, CA.

[22] "Predicting Elastic Properties of β-HMX from First-principles Calculations", Qing Peng and Suvranu De, March 4, 2015, American Physical Society (APS) March meeting, San Antonio, Texas

[23] "Pressure effect on stabilities of self-Interstitials in HCP-Zirconium", Qing Peng, Wei Ji, Jie Lian, Xiao-jia Chen, Hanchen Huang, Fei Gao, and Suvranu De, March 4, 2015, American Physical Society (APS) March meeting, San Antonio, Texas

[24] "Modeling the material strength and equations of state of beta-HMX from both first-principles calculations and molecular dynamics simulations", Qing Peng, Guangyu Wang, Gui-Rong Liu, and Suvranu De, Jun 19, 2015, 19th Biennial Conference on

Shock Compression of Condensed Matter (SCCM-2015), American Physical Society (APS) meeting, Tampa, FL

[25] "A Molecular Dynamics simulation of Hugoniot curves of HMX using ReaxFF and its application in SPH modeling of macroscale terminal effects",

[26] "van der Waals Density Functional Theory vdW-DFq for Semihard Materials", Qing Peng, Suvranu De, March 15, 2016, American Physical Society (APS) March meeting, Baltimore, Maryland, USA.

[27] "Multicale modeling of the detonation of aluminized explosives using SPH-MD-QM method", Qing Peng, Suvranu De, March 14, 2017, American Physical Society (APS) March meeting, New Orleans, Louisiana, USA.

[28] "A first-principles study of the avalanche pressure of alpha zirconium", Qing Peng, March 14, 2017, American Physical Society (APS) March meeting, New Orleans, Louisiana, USA.

Invited *Seminar* Talks

Subtotal 21

[1] "Computational Study of Localization of Plastic Shear Events in Glassy Materials", Nov 17, 2005, Geophysics Lab, Carnegie Institution of Washington, DC, USA.

[2] "Computational Study of Localization of Plastic Shear Events in Glassy Materials", Mar 20, 2006, Computational Materials Science Center in George Mason University, Fairfax, VA, USA [http://www.cmasc.gmu.edu/seminar/abstracts/peng.txt]

[3] "Materials strength at nanoscale - nanoindentation", May 17, 2008, *Science Workshop for High School Teachers*, California State University Northridge.

[4] "QCDFT:Quasi-Continuum Density Functional Theory", Sept 14, 2009, Aerospace Engineering and Mechanics, University of Minnesota, Minneapolis, MN, USA.

[5] "QCDFT:Quasi-Continuum Density Functional Theory", Sept 27, 2009, Department of Materials Science and Engineering, University of California, Los Angeles, CA, USA.

[6] "Origin of pyroelectricity in LiNbO3", Nov 6, 2009, Geophysics Lab, Carnegie Institution of Washington, DC, USA.

[7] "QCDFT:Quasi-Continuum Density Functional Theory", Oct 8, 2010, Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis, Indianapolis, IN, USA.

[8] "Quantum simulations of materials at large scale: from finite elements to electrons by QCDFT",Qing Peng, Feb 15, 2012. West Virginia University, Morgantown, WV.

[9] "Quantum simulations of materials at large scale by QCDFT",Qing Peng, Sept 27, 2012. Cardiff School of Engineering, Cardiff University, Cardiff, UK.

[10] "Quantum Simulations of Materials at Large Scale: from Finite Elements to Electrons by QCDFT Method",Qing Peng, Oct 9, 2012. Hefei National Laboratory for Physical Sciences at the Microscale, Hefei, Anhui, China. [Link]

[11] "Quantum Simulations of Materials at Large Scale", Qing Peng, Oct 21, 2013. Institute of Mechanics,Chinese Academy of Sciences, Beijing, China.

[12] "Quantum Simulations of Materials at Large Scale", Qing Peng, Oct 23, 2013. Center for applied physics and technology, Peking University, Beijing, China.

[13] "Quantum Simulations of Materials at Large Scale",Qing Peng, Oct 24, 2013. ISSP,Institute of Solid Physics,Chinese Academy of Science, Hefei, China.

[14] "Quantum Simulations of Materials at Large Scale",Qing Peng, Oct 29, 2013. Wuhan National Laboratory for Optoelectronics, Huazhong University of Science Technology, Wuhan, China.

[15] "QCDFT multiscale modeling in solid mechanics",Qing Peng, April, 2014. Washington State University, Richland, Washington, USA.

[16] "Multiscale modeling of the multi-components heterogeneous reactive systems",Qing Peng, June, 2014. Wuhan University, Wuhan, Hubei, China.

[17] "Multiscale modeling in Condensed Matter Physics",Qing Peng, Sept 16, 2015. Northeast Normal University, Jilin, China.

[18] "Multiscale modeling in Solid Mechanics",Qing Peng, Sept 21, 2015. Beijing Institute of Technology, Beijing, China.

[19] "Multiscale modeling in Condensed Matter Physics",Qing Peng, Mar 8, 2016. Albany University, Albany, USA.

[20] "QCDFT Multiscale modeling of hydrogen assisted cracking",Qing Peng, Apr 15, 2016. Institute of Coal Chemistry, Chinese Academy of Science, Taiyuan, China.

[21] "QCDFT Multiscale modeling of hydrogen assisted cracking",Qing Peng, Apr 22, 2016. Synfuels China Co. Ltd, Huairou, Beijing, China.