# Qing Peng

Dr. Qing Peng
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## Education

**University of Connecticut**, Storrs, CT
PhD, Physics (Materials Simulation), Dec 2005 (Adviser: Dr. Marcel Utz)
MS, Physics, Aug 2003
**State University of New York Binghamton**,
MS, Physics (Fluid Mechanics), 2000 (Adviser: Dr. Eric Cotts)
**Peking University**,
BS, Physics (Nuclear Science and Technology (*engineering*) ), 1998

## Conference Chair

- ⋆ American Physical Society (APS) march meeting 2013:
  Session G11: invited session: Concurrent Multi-Length Scale Modeling
- ⋆ 12th US National Congress on Computational Mechanics (USNCCM12)
  Symposium: Concurrent Multi-Length Scale Modeling: from Finite Elements to Atoms and Electrons (http://12.usnccm.org/MS4_9)
- ⋆ Asia Pacific Congress on Computational Mechanics (APCOM) 2013: Multiscale modelling and simulations: from quantum to continuum (http://www.apcom2013.org/topics–minisymposia.html)
- ⋆ 13th US National Congress on Computational Mechanics (USNCCM13)
  Symposium

## Funding Proposal Evaluator

- ♣ The research programs funded by the Romanian Government through the National Council for Scientific Research
- ♣ Romanian funding programs for research led by the National Council for Research and Development
- ♣ Executive Agency for Higher Education, Research, Development and Innovation Funding of Romanian
- ♣ National Center of Science and Technology Evaluation, Ministry of Education and Science, Republic of Kazakhstan

## Editorial Board

- ♢ "Modeling and Numerical Simulation of Materials Science"
- ♢ "Dataset Papers in Nanotechnology"

## Qing Peng

**Referee for peer reviewed journals (37)**

"Nature communications", "Nanoscale", "Physical Review B", "Physical Chemistry Chemical Physics", "Journal of Applied Physics", "The Journal of Physical Chememistry", "RSC Advances", "Modelling aand Simulation in Materials Science and Engineering", "Journal of Materials Chemistry", "Computationl Materials Science", "Journal of Elasticity", "NANO", "Journal of Physics :Condensed Matter", "Journal of Physics D: Applied Physics", "Journal of Electronic Materials", "Physics E", "Acta Materialia", "Frontiers of Physics", "IEEE Photonics Journal", "Science of Advanced Materials", "Superlattice and Microstructures", "Materials Letters", "Advances in Condensed Matter Physics", "Carbon", "Modern Physics Letters B", "IEEE J. Quantum Electronics", "European Physical Journal", "Journal of Molecular Graphics and Modelling", "World Journal of Engineering and Physical Sciences", "PLOS One", "Optical Materials", "Chemistry Central Journal", "International Journal of Thermophysics", "Journal of Optics", "Physica Status Solidi B: Basic Solid State Physics", "Nanotechnology"

**Professional Affiliations**

- American Physical Society (APS)
- Materials Research Society (MRS)
- Optical Society of America (OSA)
- United States Association for Computational Mechanics (USACM)

**Citizenship**

P.R. China

**Permanent Residence**

♠ United States of America (EB1b:Outstanding researcher)

♠ Canada (Skilled immigrants)

**Research Interests**

♡ Multiscale modeling (algorithm and applications)

♡ Nonlinear mechanics of Nanomaterials and low-dimentional materials

♡ Radiation damage

♡ Mechanics of Energetic materials

♡ Pyroelectrics and thermal energy harvesting

♡ Glasses and amorphous materials

♡ Polymer and biomaterials

# Qing Peng

## Current Research

*Postdoctoral Associate* **Rensselaer Polytechnic Institute**
Advisor:Dr. Suvranu De Jan 2011 – present

(1) Multiscale modeling (applications of QCDFT) on hydrogen embrittlement, radiation hardening, solid solution strengthening, radiation induced segregation, shear, wear, crack and corrosion of metals, especially Zr, Fe, Cu, Al, Mg; self-healing of materials after damage, such as irradiation damage and mechanical fail at high stress/strain; radiation effects on Si-based memristive devices, nano-conjunctions and interfaces; fast pipe diffusion in plasmonic metals via first-principles calculations, stabilities, diffusion and migration energies of point defects; efficiency enhancement of plasmonic solar cell by optimizing size, shape, components, layer of metal nano-particles.
(2) *ab initio* Modeling of Controlled Radiation Damage of 2D atomic crystals, such as graphene, h-BN, h-BNC, graphane, SiC, SiGe, MoS2, NbSe2, Bi2Sr2CaCu2Ox and ZnO, on electrical, thermal and mechanical properties; Surface/interface of graphene with metals and/or oxidizes, the strain, defects, diffusion and transportations;
(3) *ab initio* molecular dynamics study of elastic properties, equation of states, radiation damage process, crystal plasticity, impurities/vacancies diffusion and migration.
(4) Developing a novel multiscale QM-MD-SPH computational method for heterogeneous multicomponent reactive systems; Study the mechanical properties, equation of states, instabilities, chemical kinetics of energetic materials.
(5) Multiscale modeling and simulation the mechanics of deformation and failure of biological materials, from the atomistic (chemistry, molecular) scale up to the overall structural scale (material, tissue).

## Previous Postdoc Research Experience

*Postdoctoral Associate* Indiana Univ. Purdue Univ. Indianapolis
Advisor:Dr Guofeng Wang Jan 2010 – Dec 2010

(1)Researched in lithium-ion rechargeable batteries, especially the chemical and physical procedure on Solid electrolyte interface (SEI), which plays a critical role in the Li-ion batteries performance, including cycle life, self-discharge, safety faradaic efficiency and irreversible capacity.
(2)Conducted theoretical computations to understand and develop Pt alloy catalysts for advancing renewable energy technology.

*Postdoctoral Associate* California State Univ. Northridge
Advisor:Dr. Gang Lu Jan 2007 – Jan 2010

Developed a multiscale method named QCDFT:Quasi-Continuum Density Functional Theory, which is based entirely on density functional theory (DFT) and allows quantum simulations of materials properties of a large system with billions of atoms. QCDFT method had been successfully applied to study the nano-indentation, crack, dislocation of metals and impurities at length scales

that are relevant to experiments.

*Postdoc* Carnegie Institute of Washington
Advisor:Dr Ronald E. Cohen Jan 2006 – Dec 2006
Research in Ferroelectrics by first principles calculations and molecular dynamics simulations. The pyroelectric coefficients of $LiNbO_3$ are studied. ABINIT are used for *ab initio* calculations and DLPOLY for MD simulations. Fitted the potential for MD simulations from the *ab initio* calculations. Coded the programs that fit the force field for MD simulation from the first principle calculations.

## Graduate School Research Experience

*Research Assistant* University of Connecticut,storrs
Aug 2000 – Dec 2005
(1) Research in computer simulations of plastic deformation of polymer glasses supervised by Dr. Marcel Utz. Investigation of new approach to study localization phenomenon based on 3D Delaunay Tessellation and FFT technique. Investigated athermal simulation of plastic deformation in amorphous solids at constant pressure. Coded programs for Molecular Dynamic and Monte Carlo simulations of polymers.
(2) Conducted experimental and theoretical research on the near field diffraction of short pulse laser and quantum beat under the guidance of Dr. Chandra Roychoudhuri. Studied the dispersion of wavelength-division multiplexing (WDM) in fiber-optics communications.
(3) Facilitated experimental research on Laser Cooling and Trapping guided by Dr. Edward Eyler. Designed and built a constant-temperature diode laser system for experiments.

*Research Assistant* Binghamton University SUNY
Advisor:Dr. Eric Cotts Aug 1998 – Aug 2000
Carried experimental research on the dense suspension flow on inhomogeneous surface for under-fill flip-chip electronics packing.

## Qing Peng

TEACHING EXPERIENCE

*Teaching Assistant* **University of Connecticut**
Storrs, CT 2002 – 2005

(1) PHYS155: 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. Supervised by Dr. Cynthia Peterson.

(2) Conducted discussion sections for all fields all grades of undergraduate students in the Physics Learning Resource Center. Supervised by Dr. Carolina Artacho-Guerra.

(3) Mentor of new teaching assistants to share teaching experiences in International Teaching Assistant Program (ITAP) of UCONN (summer, 2004). Supervised by Dr. Catherine Ross.

(4) Instructed Research Undergraduate (RU) students in research of material simulation (summer,2003).

(5) Instructed Advanced High School students in research of Optics/Lasers in Photonics lab (summer, 2002).

*Mentoring Undergraduate* **RPI**
Troy, NY 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* **RPI**
Troy, NY 2012 – 2015
(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) Andrew Gaul: DFT calculations of the thermoelectrics for their mechanical and thermomechanical properties with defect engineering.

Developped Methods Software Packages

- "QCDFT", Quasi-Continuum Density Functional Theory, a concurrent multiscale method with full density functional theory calculations on macro scale. The package is coded in F90 about 8M since 2007, and it is still in development for various applications.

- "POTFIT_DLPOLY" is a DFT_MD program that fits the force field for Molecular Dynamics simulations (DL_POLY package) from first-principles DFT calculations. It is coded in Fortran, as a part of my postdoctoral research project in Carnegie Institute of Washington under the guidance of Dr. Ronald Cohen.

- "ClassicalDynamic" is a simulation package with classical Molecular Dynamics and Monte Carlo simulations by my PhD advisor Dr Marcel Utz. I coded the three-Dimensional Delaunay Tessellation for complex polymers systems applying domain decomposition and random precision techniques (coded in C++/C).

# Qing Peng

PUBLICATION LIST

(Total 43; H-index: 14; Citations: 465 –by Google Scholar[March 7, 2015])
ResearcherID: F-4246-2010; ORCID:0000-0002-8281-8636

**Refereed Journal Articles** (37; average Impact Factor (IF):2.831)
* 31 of 37 are *first-* and *corresponding* authored

(1) **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]

(2) 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, Pyrotechnicsa (2015), published online, DOI: 10.1002/prep.201400244 [link]

(3) **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. (IF=4.198) [link]

(4) **Q. Peng*** and S. De, "Elastic limit of silicane", *Nanoscale*,(2014), **6**, 12071–12079 (IF=6.739) [link]

(5) **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. (IF=4.198) [link]

(6) **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). (IF=5.078) [link]

(7) **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). (Editor Invited Review) [link]

(8) 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]

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

(10) Y. Sun, **Q. Peng**, and G. Lu, "Quantum Mechanical Modeling of Hydrogen Assisted Cracking in Aluminum", *Physical Review B*, **88** 104109 (2013).

[link]

(11) **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). (IF=4.198) [link]

(12) **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). (Editor Invited Review) [link]

(13) **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*, (2013), Articles ASAP, DOI: 10.1080/15376494.2013.839067. [link]

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

(15) **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]

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

(17) **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]

(18) **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]

(19) **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]

(20) **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). (IF=4.198). [link]

(21) **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). (IF=6.739). [link]

(22) **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]

(23) **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]

(24) **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]

(25) **Q. Peng*** , W. Ji, and S. De, "Mechanical Properties of Graphyne Monolayer: A First-Principles Study", *Physical Chemistry Chemical Physics*, **14**, 13385–13391 (2012). (IF=4.198) [link]

(26) **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]

(27) **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]

(28) **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]

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

(30) **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). ("Featured Articles" in Advances In Engineering) (IF=4.289), [link]

(31) 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]

(32) 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]

(33) **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]

(34) **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]

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

(36) **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). (Editors' Suggestion) [link]

(37) 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]

## Peer-reviewed Conference Proceedings (full paper) (4)

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

(2) **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]

(3) 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]

(4) 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]

## Books and/or Book Chapters (2)

(1) **Q. Peng**, "First-Principles Quantum Simulations", Chapter 1 in book "Nanoindentation in Materials Science", edited by Jiri Nemecek. (2012) In-TechOpen, 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", Chap-

ter 34 in book “Graphene Science Handbook”, Vol 4 “Mechanical and Chemical Properties”, edited by Z.A. Niknam. (2015) CRC Press/Taylor & Francis. [local PDF]