

Qing Peng

Dr. Qing Peng
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EDUCATION

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

PROFESSIONAL ACTIVITIES

- Reviewer of “Physical Review B”, “Computational Materials Science”, “Journal of Elasticity” and “Modelling and Simulation in Materials Science and Engineering”
- Expert evaluator of the research programs funded by the Romanian Government through the National Council for Scientific Research.
- Expert evaluator of Romanian funding programs for research led by the National Council for Research and Development.

CURRENT RESEARCH

Postdoctoral Associate **Rensselaer Polytechnic Institute**
Advisor: Dr. Suvranu De Jan 2011 – present
(1) Multiscale modeling (applications of QCDFDFT) 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, Bi₂Sr₂CaCu₂O_x 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.

PREVIOUS
RESEARCH

Postdoctoral Associate

**Purdue School of Eng Tech
IUPUI**

Jan 2010 – Dec 2010

Advisor: Dr Guofeng Wang

(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 University
Northridge**

Jan 2007 – Jan 2010

Advisor: Dr. Gang Lu

Developed a multiscale method named QCDFE: 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. QCDFE 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 Inst. of Washington

Jan 2006 – Dec 2006

Advisor: Dr Ronald E. Cohen

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.

Research Assistant

University of Connecticut, Storrs

Aug 2000 – Dec 2005

Advisor: Dr Marcel Utz

(1) Research in computer simulations of plastic deformation of polymer glasses. 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. Studied the dispersion of wavelength-division multiplexing (WDM) in fiber-optics communications.

(3) Facilitated experimental research on Laser Cooling and Trapping. Designed and built a constant-temperature diode laser system for experiments.

Research Assistant

**Sate University of New York
Binghamton**

Aug 1998 – Aug 2000

Advisor: Dr. Eric Cotts

Carried experimental research on the dense suspension flow on inhomogeneous surface for under-fill flip-chip electronics packing.

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TEACHING EXPERIENCE

Teaching Assistant
Storrs, CT

University of Connecticut
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
Troy, NY

RPI
2011 – present

- (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.

- (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.

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FUNDING
PROPOSAL
EXPERIENCE

Nuclear Energy University Programs, DOE

PI: Suvrana De Co-PI: Hanchen Huang 2011
My role: *helped for preparation* status: *pending*
“Multiscale Modeling of the Effects of Neutron Irradiation on the Mechanical Properties of HCP metals”
Amount: \$ 849K (3 years)

Defense Threat Reduction Agency, DOD

PI: Suvrana De 2011
My role: *helped for preparation* status: *pending*
“Temperature and strain-rate dependent mechanical properties of graphene”
Amount: \$ 300K (3 years)

Defense Threat Reduction Agency, DOD

PI: Suvrana De Co-PI: Saroj Nayak 2011
My role: *helped for preparation* status: *pending*
“Investigating the Effects of Radiation on the Mechanical Response of Memristors Based on Novel Multiscale Computational Techniques”
Amount: \$ 800K (3 years)

European Research Council Starting Grants 2011

Host: Cardiff University, UK 2010
My role: *PI* Status: *Not funded*
“Quasi-Continuum Density Functional Theory”
Amount: £ 2M (5 years)
Cardiff University is the host institution in this grant application, offering lecture position only if the grant get funded.

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PUBLICATIONS

BOOK CHAPTERS

- (1) **Q. Peng**, “Quantum mechanical simulations of nanoindentation”, in book “Nanoindentation”, edited by Jiri Nemecek. To be published in April 2012, by InTechOpen.
ISBN 980-953-307-282-6.

MANUSRIPTS IN PREPARATION

- (1) **Q. Peng**, M. Rose, and R.E. Cohen, “Origin of Electrocaloricity in Lithium Niobate”.
- (2) Y. Sun, **Q. Peng** and G. Lu, “Hydrogen embrittlement at Al Crack Tip: A multiscale study”.
- (3) **Q. Peng**, W. Ji and S. De, “Hydrogen diffusion along twin boundary of hcp-Zr”.
- (4) **Q. Peng**, W. Ji, J. Lian and S. De, “First-principles phonon calculations of thermal properties of Uranium Carbide”.
- (5) **Q. Peng**, C. Huang, I. Shin, E. A. Carter and S. De, “Persitation in Al-Mg alloy: ab initio calculations over million elections”.
- (6) **Q. Peng**, W. Ji, J. Lian and S. De, “Hydrogen embrittlement in bcc-Zr: A QCDFT application”.
- (7) **Q. Peng**, W. Ji, J. Lian and S. De, “First-principles Phonon Calculations of Thermal Properties of Iron: Nudged Quantum Harmonic Approximation Method”.
- (8) **Q. Peng**, W. Ji, S. Bordas and S. De, “Silicon embrittlement at Al Crack Tip: A multiscale study”.

ARTICLES UNDER REVIEW

- (1) **Q. Peng**, W. Ji and S. De, “Tunable Band Gaps of Mono-layer Hexagonal BNC Heterostructures”, Submitted to PRL, in revising. [[arXiv:1105.3776v1](https://arxiv.org/abs/1105.3776v1)]

- (2) **Q. Peng**, W. Ji, A. R. Zamiri and S. De, “Elastic Properties of Hybrid Graphene/Boron Nitride Monolayer”, submitted to Computational Materials Science, in revising. [[arXiv:1107.1448](#)]
- (3) **Q. Peng**, Z. Duan and G. Wang, “First Principles Study of Lithium Diffusion during Intercalation into Graphite”, submitted to Journal of Physics D: applied physics, in revising. (Manuscript is available by request).
- (4) **Q. Peng**, Z. Duan and G. Wang, “Computational Studies of the Initial Reduction and Adsorption Mechanisms of Ethylene Carbonate on the Surface of Carbon Anodes”, Submitted to Surface Science, in revising (Manuscript is available by request).
- (5) **Q. Peng**, M. Utz, “Deformation Dilatancy of Molecular Glasses”, Submitted to Phys. Rev. E, in revising. [[arXiv:1110.6699](#)]
- (6) **Q. Peng**, W. Ji and S. De, “Strain effect on Controlled Radiation Damage: ab initio Modeling of Mono-layer Hexagonal Boron Nitride”, Submitted to ACS nano (Manuscript is available by request).
- (7) **Q. Peng**, W. Ji and S. De, “ab initio Study of Concentration Effect on the Stabilities of Point Defects in hcp-Zirconium”, Submitted to Philosophical Magazine (Manuscript is available by request).
- (8) **Q. Peng**, W. Ji, J. Lian and S. De, “First-principles phonon calculations of thermal properties of hcp, ω , bcc and fcc Zirconium”, Submitted to J. of Physics: Condensed Matter (Manuscript is available by request).

PEER-REVIEWED JOURNAL ARTICLES

- (9) **Q. Peng** W. Ji and S. De, “Mechanical Properties of the Hexagonal Boron Nitride Monolayer: ab initio Study”. Computational Materials Science (2011). [[DOI:10.1016/j.commatsci.2011.12.029](#)]
- (10) **Q. Peng** and R.E. Cohen, “Origin of Pyroelectricity in LiNbO₃”. Phys. Rev. B 83, 220103(Rapid communication) (2011). [[PDF](#)]
- (11) **Q. Peng** and G. Lu, “A comparative study of fracture in Al: quantum mechanical vs. empirical atomistic description”, J. of Mechanics and Physics of Solid, 59 (2011) page 775–786. [[PDF](#)]
- (12) Y. Zhao, **Q. Peng** and G. Lu, “Error Analysis and Applications of a General QM/MM Approach”, Comput. Mater. Sci., 50, 714 (2010), [[PDF](#)]
- (13) X. Zhang, **Q. Peng** and G. Lu, “Self-consistent embedding quantum mechanics/molecular mechanics method with applications to metals.”, Phys.

Rev. B, 82,134120 (2010) [[PDF](#)]

(14) **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 Simul. Mater. Sci. Eng.*, 18, 075003 (2010) [[PDF](#)]

(15) **Q. Peng**, X. Zhang and G. Lu, “Structure, mechanical and thermodynamic stability of vacancy clusters in Cu”, *Modelling Simul. Mater. Sci. Eng.*, 18, 055009 (2010) [[PDF](#)]

(16) **Q. Peng**, X. Zhang, and G. Lu, “Quantum mechanical simulations of nanoindentation of Al thin film”, *Comput. Mater. Sci.*, 47, 769 (2010) [[PDF](#)]

(17) **Q. Peng**, X. Zhang, L. Hung, E. A. Carter and G. Lu, “Quantum Simulation of Materials at Micron Scales and Beyond”, *Phys. Rev. B*, 78, 054118 (2008). (Editors’ suggestion) [[PDF](#)]

(18) M. Utz, **Q. Peng** and M. Nandagopal, “Athermal simulation of plastic deformation in amorphous solids at constant pressure”, *Journal of Polymer Science B: Polymer Physics* 42 (11): 2057-2065 JUN 1 (2004) [[PDF](#)]

CONFERENCE AND PROCEEDINGS ARTICLES

(1) G. Lu, **Q. Peng**, X. Zhang, L. Hung and E. A. Carter, Oberwolfach Reports, Volume 5, Issue 2, 1117 (2008) [[PDF](#)]

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

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PRESENTATIONS

INVITED TALKS

- (1) “Computational Study of Localization of Plastic Shear Events in Glassy Materials”, Oct 17, 2005, Geophysics Lab, Carnegie Institution of Washington, DC
- (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 [[Link](#)]
- (3) “QCDFT:Quasi-Continuum Density Functional Theory”, Sept 14, 2009, Aerospace Engineering and Mechanics, University of Minnesota.
- (4) “QCDFT:Quasi-Continuum Density Functional Theory”, Sept 27, 2009, Department of Materials Science and Engineering, UCLA.
- (5) “Origin of pyroelectricity in LiNbO₃”, Nov 6, 2009, Geophysics Lab, Carnegie Institution of Washington, DC.
- (6) “QCDFT:Quasi-Continuum Density Functional Theory”, Oct 8, 2010, Department of Chemistry and Chemical Biology, IUPUI.

CONFERENCE PRESENTATIONS

- (1) “Computer Simulation of The Localization of Plastic Shear Events in Molecular Glasses”, Qing Peng, Marcel Utz, March 30, 2005, 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, APS March Meeting, Los Angeles, CA [[Link](#)]
- (3) “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
- (4) “First Principle Based Computation of Pyroelectricity in LiNbO₃”, Q. Peng, R. E. Cohen, March 18,2010, APS March Meeting, Portland, OR [[Link](#)]
- (5) “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 [[Link](#)]

(6) “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.

(7) “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 [[Link](#)]

(8) “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

(9) “A QCDFEFT Study of Hydrogen embrittlement at Crack Tip”, Qing Peng, Mar 22, 2011, APS March Meeting, Dallas, TX. [[Link](#)]

(10) “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.

(11) “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.

(12) “An Accelerated Quasicontinuum-DFT (QCDFEFT) 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.

(13) “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.

(14) “Hydrogen Embrittlement in Zirconium: a Quasi-Continuum Density Functional Theory Study”, Qing Peng, Feb 27, 2012. APS meeting, Boston, MA.

(15) “Golden Rule of Radiation Hardness: a Study of Strain Effect on Controlled Radiation Damage”, Qing Peng, Mar 1st, 2012. APS meeting, Boston, MA.

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ADMINISTRATOR EXPERIENCE

Systems Administration, **Rensselaer Polytechnic Institute**
Department MANE
Troy, NY 2011 – present
Administration of a 27 Teraflops super computer (about 500 cores with infiniband) for high performance scientific computation. Daily maintenance of the cluster in both hardware and software. Webpage: <http://neams.rpi.edu>

Systems Administration, **Cal. State Univ. Northridge**
Keck Lab of Physics Department
Northridge, CA 2008 – 2010
Designed and built a 2.0 Teraflops supper computer (200 cpus) for high performance scientific computation from scratch, including ordering each component (motherboard, memory,cpu,case,fan, etc) and assembled them onto the cluster. Installed the operation system and application software with daily maintenance thereafter.

Systems Administration, **University of Connecticut**
Computer Lab of Physics Department
Storrs, CT 2003 – 2005
Daily maintenance of computers in the Computer Lab of the Physics Department, including hardware repair/replacement, software installation/updating, daily virus and security checking and updates.
Providing solutions of all problems related to computers, emails, internet connection, printer connection, scanner usage, printing etc. Supervised by Dr. Michael Rozman.

Systems Administration, **University of Connecticut**
Institute of Material Science
Maintained a parallel computing 30 nodes Beowulf cluster which permits state-of-the-art computer simulation to analyze and predict the behavior of metal, polymer, ceramic and composite materials under diverse conditions. Supervisor: Dr. Marcel Utz.

PROFESSIONAL AFFILIATIONS

- American Physical Society (APS)
- Materials Research Society (MRS)
- Optical Society of america (OSA)

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SOFTWARE PACKAGES

- “QCDFIT”, Quasi-Continuum Density Functional Theory, a concurrent multiscale method with full density functional theory calculations on macro scale. The package is coded in F90, and still in heavy developing for various applications, since 2007. The source code size is about 6M.
- “POTFIT”, a program fits the force field for MD simulation from first-principles DFT calculations. It is coded in Fortran.
- “ClassicalDynamic” is a simulation package with Molecular Dynamics and Monte Carlo simulations. I coded the three-Dimensional Delaunay Tessellation for complex polymers systems applying domain decomposition and random precision techniques. It is coded in C++/C.