

Qing Peng

Dr. Qing Peng
Rensselaer Polytechnic Institute
110 8th Street, JEC 2303
Troy, NY 12180

Web <http://qpeng.org>
Email pengq3@rpi.edu
Cell: (518) 279-6669
Fax: (518) 276-6025

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

- Editorial Board: “Modeling and Numerical Simulation of Mater. Sci.”
- Editorial Board: “Dataset Papers in Nanotechnology”
- Reviewer: “Physical Review B”, “Computational Materials Science”, “Journal of Elasticity”, “NANO”, “J. Applied Physics”, “J. Physics:Condensed Matter”, “J. Electronic Materials”.
- 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
Advisor: Dr. Suvranu De

Rensselaer Polytechnic Institute

Jan 2011 – present

(1) Multiscale modeling (applications of QCDFE) 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

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 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

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.

Research Assistant

University of Connecticut, Storrs

Advisor: Dr. Marcel Utz

Aug 2000 – Dec 2005

(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

Binghamton Univ. 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 packaging.

BOOK CHAPTERS

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

ARTICLES UNDER REVIEW

- (1) **Q. Peng**, W. Ji, H. Huang and S. De, “Strain Effect on the Stability of Self-interstitials in hcp-Zr”, Submitted to PRL.
- (2) **Q. Peng**, W. Ji, X. Chen, and S. De, “Mechanical Failure of Hexagonal Boron Nitride Monolayer”, Submitted to PRB.
- (3) **Q. Peng**, W. Ji and S. De, “Effect of Pressure on the Stability of Self-Interstitials in hcp-Zr”, Submitted to PRB.
- (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.
- (5) **Q. Peng**, M. Utz, “Deformation Dilatancy of Molecular Glasses”, Submitted to Phys. Rev. E, [[arXiv:1110.6699](https://arxiv.org/abs/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.
- (7) **Q. Peng**, W. Ji, H. Huang and S. De, “Stability of Self-interstitials in hcp-Zr”, Submitted to J. Nucl. Mater.
- (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.
- (9) Y. Sun, **Q. Peng**, and G. Lu, “Hydrogen assisted cracking: a QCDFD study of Aluminum crack-tip”, Submitted to PRB.
- (10) **Q. Peng**, W. Ji, H. Huang, X. Chen, and S. De, “Monovacancy in hcp-Zirconium”, Submitted PRB.

(11) **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 Modeling and Numerical Simulation of Material Science.

(12) **Q. Peng**, “Localization of Plastic Relaxation Events in Glassy Materials”, Submitted.

PEER-REVIEWED JOURNAL ARTICLES

(1) **Q. Peng**, A. R. Zamiri, W. Ji, and S. De, “Elastic Properties of Hybrid Graphene/Boron Nitride Monolayer”, Acta Mechanica, in press.
also: [[arXiv:1107.1448](https://arxiv.org/abs/1107.1448)]

(2) **Q. Peng**, and S. De, “Tunable Band Gaps of Mono-layer Hexagonal BNC Heterostructures”, Physica E: Low-dimensional Systems and Nanostructures, in press. [[DOI:10.1016/j.physe.2012.04.011](https://doi.org/10.1016/j.physe.2012.04.011)]

(3) **Q. Peng**, W. Ji and S. De, “Mechanical Properties of the Hexagonal Boron Nitride Monolayer: ab initio Study”. Comput. Mater. Sci. 56, 11 (2012). [[PDF](#)]

(4) **Q. Peng** and R.E. Cohen, “Origin of Pyroelectricity in LiNbO₃”. Phys. Rev. B 83, 220103(Rapid communication) (2011). [[PDF](#)]

(5) **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](#)]

(6) Y. Zhao, C. Wang, **Q. Peng** and G. Lu, “Error Analysis and Applications of a General QM/MM Approach”, Comput. Mater. Sci., 50, 714 (2010), [[PDF](#)]

(7) 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](#)]

(8) **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](#)]

(9) **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](#)]

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

(11) **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](#)]

(12) 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

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

(14) **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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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.