

Qing Peng

Dr. Qing Peng
Department of Mechanical Engineering
Purdue School of Engineering
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EDUCATION

University of Connecticut, Storrs, CT
PhD, Physics (Materials Simulation), Oct 2005
Dissertation: “Localization of Plastic Shear Events in Glassy Materials”
Adviser: Dr. Marcel Utz

University of Connecticut, Storrs, CT
MS, Physics (Materials Simulation), Aug 2003
Adviser: Dr. Marcel Utz

State University of New York, Binghamton, NY
MS, Physics (Fluid Mechanics), Aug 2000
Thesis: “A Study of the Flow of Dense Suspension on Inhomogeneous Surfaces”
Adviser: Dr. Eric Cottis

Beijing University, Beijing, China
BS, Physics (Nuclear Science and Technology), Jun 1998
Thesis: “Analytically Solve Dirac Equation with SU(3) Algebra”
Adviser: Dr. Hua Guo

CURRENT RESEARCH

Postdoctoral Associate
Mechanical Engineering
Indianapolis, IN

**Purdue School of Engineering and
Technology**
Jan 2010 – present

Research 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.

Conduct theoretical computations to understand and develop Pt alloy catalysts for advancing renewable energy technology.

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PUBLICATIONS

- (14) **Q. Peng**, and S. Bordas, “Quantum mechanical simulations in Prediction of Crack Tip Dislocation Nucleation at Micron scale”, in preparing.
- (13) **Q. Peng**, Z. Duan and G. Wang, “First Principles Study of Lithium Diffusion during Intercalation into Graphite”, in preparing.
- (12) **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 *Journal of Physics D*, applied physics.
- (11) Y. Zhao, **Q. Peng** and G. Lu, “Magnetism-driven dislocation mobility in NiAl: A QM/MM study.” submitted to PRB
- (10) **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.*, in press
- (9) **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*, in press (also arXiv:0907.3572v1)
- (8) X. Zhang, **Q. Peng** and G. Lu, “QM/MM methodology based on OFDFT with applications on metals.”, PRB, in press
- (7) **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)
- (6) **Q. Peng**, X. Zhang, and G. Lu, “Quantum mechanical simulations of nanoindentation of Al thin film”, *Comput. Mater. Sci.*, 47, 769 (2010)
- (5) **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**, 9 (2009).
- (4) G. Lu, **Q. Peng**, X. Zhang, L. Hung and E. A. Carter, *Oberwolfach Reports*, Volume 5, Issue 2, 1117 (2008)
- (3) **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).
- (2) Q. Peng and R.E. Cohen, “Pyroelectricity in Lithium Niobate”. submitted to PRL.
- (1) 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)

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PRESENTATIONS

Talk on “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](#)]

Talk on “First Principle Based Computation of Pyroelectricity in LiNbO₃”, Q. Peng, R. E. Cohen, March 18, 2010, APS March Meeting, Portland, OR [[Link](#)]

Talk on “What can we learn by differentiating between the physical processes behind interference and diffraction phenomena?”, Qing Peng, Michael A. Barrootkoob, Chandrasekhar Roychoudhuri, Aug 3, 2009, SPIE Meeting, San Diego, CA [[Link](#)]

Invited talk on “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](#)]

Talk on “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](#)]

“Computer Simulation of The Localization of Plastic Shear Events in Molecular Glasses”, Qing Peng, Marcel Utz, March 30, 2005, MRS Spring Meeting, San Francisco, CA

PREVIOUS
RESEARCH

Postdoctoral Associate
Physics Department
Northridge, CA

California State University

Jan 2007 – Jan 2010

Research in development and applications of a DFT-based quasicontinuum method (QCDFE). QCDFE can simulate multimillion atoms effectively via density functional theory without empirical input to the energetics formulation. This method had been successfully applied to study the nano-indentation, crack, dislocation of metals and impurities. This method represents a new direction for the quantum simulation of materials at length scales that are relevant to experiments.

Carried out detailed study of atomic structure, mechanical and thermodynamic stability of vacancy clusters by atomistic simulations; a comparative study of fracture in Al by using quantum mechanical and empirical atomistic description of atomic interaction at crack tip; a novel magnetism-driven dislocation motion and cross-slip in NiAl alloys.

Object: Multiscale (QCDFE)

Method: *ab initio* and MD simulations

Advisor: Dr. Gang Lu

Postdoctoral Associate
Geophysical Laboratory
Washington, DC

**Carnegie Institution of
Washington**

Jan 2006 – Dec 2006

Research in computer simulations of Ferroelectrics using first principle and molecular dynamics methods. The pyroelectric coefficients of LiNbO_3 are studied. The programs used are ABINIT for *ab initio* calculation and DLPOLY for MD simulations. Fitting the potential for MD simulations from the *ab initio* calculations. Coding the programs that fit the force field for MD simulation from the first principle calculations.

Object: Ferroelectrics (LiNbO_3)

Method: *ab initio* and MD simulations

Advisor: Dr. Ronald E. Cohen

Research Assistant
Physics and Material Science
Storrs, CT

University of Connecticut

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. Coding programs for Molecular Dynamic and Monte Carlo simulations of polymers.

Object: polymer glasses

Method: MD and MC simulations (classical)

Advisor: Dr. Marcel Utz

(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
Cotts Lab
Binghamton, NY

Sate University of New York

Aug 1998 – Aug 2000

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

Object: dense suspension fluid (Dexter)

Method: Capillary flow

Advisor: Dr. Eric Cotts

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 quiz, mid-term exams and finals. Supervised by Dr. Cynthia Peterson.

(2) Conduct discussion sections for all fields all grades of undergraduate students in 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) Instruction Research Undergraduate (RU) students in research of material simulation (summer, 2003).

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

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ADMINISTRATOR EXPERIENCE

Systems Administration, **Cal. State Univ. Northridge**
Keck Lab of Physics Department
Northridge, CA 2009 – present
Designed and builded 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. Daily maintaining the cluster in both hardware and running status.

Systems Administration, **University of Connecticut**
Computer Lab of Physics Department
Storrs, CT 2003 – 2005
Daily maintain of computers in the Computer Lab of the Physics Department, including hardware repairing/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 using, printing etc. Supervised by Dr. Michael Rozman.

Systems Administration, **University of Connecticut**
Institute of Material Science
Maintaining 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.

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SKILLS

ab initio

CALCULATION SKILLS

Four years experience with VASP and ABINIT to do geometry optimization, calculate Band structure, Charge densities, Born effective Charge, Phonon dispersion, Vibrational properties, Elastic constants, Pyroelectric constants, Thermal expansion, Heat capacity, etc.

CLASSICAL SIMULATION SKILLS

Developed our own code to perform Molecular Dynamics (MD) Simulation, Monte Carlo (MC) Simulation, Simulated Annealing, Plastic deformation simulation, 3D Delaunay Tessellation. Familiar with LAMMPS and DLPOLY to carry out various applications.

MULTISCALE CONTINUUM SIMULATION SKILLS

Developed our own code (QCDFE) to perform the multiscale simulations which expands varies scales (from continuum Macroscale to atomic) and principles (from elastic to quantum mechanics). Familiar with FEM methods for modeling and computation.

QUANTITATIVE SKILLS

Matlab calculation and modeling, mathematical modeling, probability, statistics, numerical methods, finite difference method, finite element method, stochastic differential equations, PDE, Monte Carlo methods, signal/data processing, linear and nonlinear filtering, parameter estimation, time series analysis, principal component analysis

COMPUTER SKILLS

- Expert knowledge of the programming languages: C++/C/F, Python, PHP, Matlab, Mathematica and HTML.
- Expert knowledge of the Linux operating system and related applications.
- Expert knowledge of the winxp/win2000/win98 operating system and related applications.
- Expert knowledge of the databased driven website design.

EXPERIMENT SKILLS

- **Certified** Machine shop working skills by School of Engineering of Uconn.
- Expert at optics/laser experiment.
- Expert at capillary flow/rheology experiment.
- Advanced knowledge of the solid state NMR experiment.

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REFERENCES

Please contact my references for your serious consideration.

- PostDoc supervisor
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- PostDoc supervisor
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California State University Northridge
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- PhD advisor
Marcel Utz, Dr. sc. techn. ETH
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University of Virginia
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- Optics Research advisor
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