Dr. Qing Peng

Physics Department, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia
Saudi: qing.peng@kfupm.edu.sa +966(13)8601797 qpeng.org@gmail.com +1(518)3003668

Education

2005	Ph.D.	Physics, University of Connecticut, Storrs, CT, U.S.A.
2000	M.S.	Physics, State University of New York, Binghamton, NY, U.S.A.
1998	B.S.	Physics, Peking University, Beijing, China

Professional Positions

2020.1–	Associate Professor, KFUPM, Saudi Arabia
2020.10–	KACARE Research Fellow, Energy Research & Innovation Center at Dhahran, Dhahran, Saudi Arabia
2020.6–	Coordinator, Master of *Computational Materials and Modeling*, KFUPM
2020.5–	Founder, Pyrosolar, Dhahran, Saudi Arabia
2016-2019	Research Fellow, University of Michigan, Ann Arbor,MI,USA
2011-2016	Postdoctoral researcher, Rensselaer Polytechnic Institute, Troy, NY, USA
2010	Postdoctoral Research Associate, Indiana Univ Purdue Univ Indianapolis
2007-2010	Postdoctoral researcher, California State University Northridge,CA,USA
2006	Postdoctoral researcher, Carnegie Institute of Washington, DC, USA

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

Current Research supports

- K.A.CARE Research Fellowship, "First-principles Investigation on Anode Performance of Naooegg Graphene for Sodium Ion Batteries", Amount: **SAR$ 120 K**, 2020-2021. *note: PI*
- Deputyship for Research and Innovation, KSA international research collaboration grant, "Towards Solar Energy Harvesting in KSA: Revisiting Deep Eutectic Solvents Using Coordination Chemistry to Synthesize New Inorganic-Organic Hybrids with Charge-Transport Properties", Total amount: **SAR$7M**, 2020-2023 (Three years). *note: Co-PI.*

- KAUST Supercomputing Laboratory, "Atomistic study on anode performance of nanoegg graphene for sodium ion batteries", Amount: 2.3 million-core-hours computation resources (Equivalent grant of **USD$30K**). 2020-2021 (1 year). *note: PI*
- Deanship of Research, KFUPM, "Atomistic study of the shock physics of the nanoegg graphene", Amount: **SAR$ 82.5K**, 2020-2021. *note: PI*

Group members/Current students

- Postdocs: Ismail Abdulazeez, Hamisu Aliyu Mohd
- PhD students: Chidera Churchill NNadiekwe, Muhammad Hanif, Mustapha Umar, Yusron Darojat, Al-iwowiyy Adeyeye
- Master students: Sameh M.A. Altanany
- Undergraduates: Ishaq Ibrahim Alahmed, Emad Aboud Alharthi, Saeed Alsurki

Editor

1. Associate Editor of Applied Physics Reviews (IF 17.054)
2. Topic Editor of Frontiers in Chemistry (IF 3.693)
3. Topic Editor of Frontiers in Nanotechnology (IF 3.9)
4. Guest Editor of Crystals (IF 2.061)
5. Guest Editor of Journal of Composites Science
6. Guest Editor of Nanophotonics (SPIE)

Editorial Board

1. Scientific Reports (IF 4.011)
2. Crystals (IF 2.404)
3. Frontiers in physics (IF 2.470)
4. Graphene
5. Current Graphene Science
6. Modeling and Numerical Simulation of Materials Science

Conference Chair

1. 12th International Conference on Computational Methods, Vietnam 2021 (ICCM2021), July 4th-8th, Vietnam
2. 11th International Conference on Computational Methods, Vietnam 2020 (ICCM2020), July 7th-11th, Vietnam
3. 10th International Conference on Computational Methods, Singapore 2019 (ICCM2019), July 9th-13th
4. The 18th US National Congress for Theoretical and Applied Mechanics (USNCTAM) Symposium, Northwestern University, Evanston, IL, USA,2018

5. The 14th US National Congress on Computational Mechanics (USNCCM14) Symposium, Montreal, Canada,2017 (http://14.usnccm.org)
6. The 8th International Conference on Computational Methods (ICCM2017), Guilin,China,2017 (http://www.sci-en-tech.com/ICCM/index.php/iccm2017)
7. The 17th International Conference on Electronic Packaging Technology (ICEPT 2016) Wuhan, China, Aug 16-19 2016 (http://www.icept.org/en)
8. The 13th US National Congress on Computational Mechanics (USNCCM13) Symposium, San Diego, CA, USA, 2015
9. American Physical Society (APS) march meeting 2013: Session G11: Concurrent Multi-Length Scale Modeling, Baltimore, MD, 2013
10. 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
11. Asia Pacific Congress on Computational Mechanics (APCOM) 2013: Multiscale modelling and simulations: from quantum to continuum, Singapore, 2013

Grant Panels

1. OPUS,National Science Center, Poland, 2018
2. Consolidated Innovative Nuclear Research (NEUP/NEET/NSUF), Department of Energy, United States, 2017,2018,2019,2020
3. National Center of Science and Technology Evaluation, Ministry of Education and Science, Republic of Kazakhstan, 2015,2017,2018,2019
4. Executive Agency for Higher Education, Research, Development and Innovation Funding of Romanian,2014,2015,2020
5. Romanian funding programs for research led by the National Council for Research and Development,2013
6. The research programs funded by the Romanian Government through the National Council for Scientific Research, 2012

SERVICES

- Coordinator for Undergraduate Research, Department of Physics, King Fahd University of Petroleum and Minerals, 2020-2021.
- Coordinator for Professional Mater program of Computational Materials and Modeling, Department of Physics, King Fahd University of Petroleum and Minerals, 2020-2021.
- Coordinator for Professional Concentration program of Computational Materials and Modeling, Department of Physics, King Fahd University of Petroleum and Minerals, 2020-2021.
- Faculty Search Committee, Department of Physics, King Fahd University of Petroleum and Minerals, 2020-2021.
- MSE Program Committee, King Fahd University of Petroleum and Minerals, 2020-2021.

- MSE Task Force Committee, King Fahd University of Petroleum and Minerals, 2020-2021.

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)
- Royal Society of Chemistry Member (MRSC)

Honors

- "K.A.CARE Research Fellowship", Saudi Arabic, 2020
- "Chutian Scholar", Hubei Province, China, 2017
- Honoree of the 44th Annual Service Recognition, Rensselaer Polytechnic Institute, 2016

Recent Grants and Awards

1. Award, K.A.CARE Research Fellowship, KSA
2. Grant from Deputyship for Research and Innovation,KSA, SAR $7M for three years, 2020-2023.
3. Grant from DSR, King Fahd University of Petroleum and Minerals, SAR $82.5K for one year, 2020-2021.
4. Grant from KAUST Supercomputing Laboratory, USD $30K for one year, King Abdullah University of Science and Technology, 2020-2021,
5. Nominee for "Blavatnik Award for Young Scientists" by Rensselaer Polytechnic Institute, 2016
6. The 6th most cited Computational Materials Science articles published since 2011
7. Granted participant of "Gordon Research Seminar" on Energetic Materials, June 14-15, Newry, ME, 2014

Invited reviewer for Journals (70)

(1)Nature Communications, (2)Physical Review Letters, (3)Advanced Materials, (4)Nano Letters, (5)Nanoscale, (6)Physical Review Materials, (7)Acta Materialia, (8)Physical Chemistry Chemical Physics, (9)The Journal of Physical Chemistry, (10)2D Materials, (11)Chemistry of Materials, (12)Physical Review B, (13)Journal of Materials Chemistry, (14)Computational Materials Science, (15)Journal of Applied Physics, (16)Journal of Physics :Condensed Matter, (17)Journal of Physics D: Applied Physics, (18)Journal of Electronic Materials, (19)Materials Characterization, (20)Journal of Elasticity, (21)Physics E, (22)Chemical Physics Letters, (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)Materials Horizons, (34)Nano Energy, (35)Optical Materials, (36)Chemistry Central Journal, (37)International Journal of Thermophysics, (38)Materials and Design, (39)Physica Status Solidi B: Basic Solid State Physics, (40)Nanotechnology, (41)Journal of Computational Chemistry, (42)RSC Advances, (43)Surface Review and Letters, (44)Modelling and Simulation in Materials Science and Engineering, (45)International Journal of Quantum Chemistry, (46)The Journal of Experimental Nanoscience, (47)Journal of Spacecraft and Rockets, (48)Physical Review A, (49)Engineering Fracture Mechanics, (50)Nano Today, (51)Journal of Materials Research, (52)Journal of Vacuum Science and Technology A, (53)Journal of Geophysics and Engineering, (54)Diamond and Related Materials, (55)Journal of Micromechanics and Molecular Physics, (56)Journal of Energetic Materials, (57)International Journal of Hydrogen Energy, (58)Current Applied Physics, (59)Computational Condensed Matter, (60)Results in Physics, (61)Journal of Materials Science and Nanotechnology, (62)The European Physical Journal Plus, (63)International Journal of Recent advances in Mechanical Engineering, (64)PLOS One, (65)Optical Express, (66)World Journal of Engineering and Physical Sciences, (67)NANO, (68)Journal of Optics, (69)Frontiers of Physics, (70)npj 2D Materials,

TEACHING

Teaching Course
Associate Professor KFUPM
Dhahran 31261, Saudi Arabia 2020,2021
PHYS630: Phase Transitions and Critical Phenomena
Theoretical study of phase transitions and critical phenomena: (3 credits)
Topics covered include: Introduction to the main characteristics of phase transition phenomena; Simple models (Ising, Gaussian and spherical models); real space renormalization; mean field theory, Landau-Ginzburg model; diagrammatic perturbation theory and Feynman rules in wave vector space; renormalization group theory; applications.
Prerequisites: PHYS530 (Stattistical Mechanics)

2021

PHYS619: Projects
(3 credits)
Description: A required course for Professional Master of Computational Materials and Modeling.
A graduate student will arrange with a faculty member to conduct an industrial research project related to the QIC, the field of the study. Subsequently the students shall acquire skills and gain experiences in developing and running actual industry-based project. This project culminates in the writing of a technical report, and an oral technical presentation in front of a board of professors and industry experts.

2020,2021

PHYS531: Monte Carlo Simulations in Statistical Mechanics
(3 credits)
Description: Review of pertinent topics in classical and quantum physics. Gibb's statistical ensembles, MB, BE, and FD statistics with simple applications to solids. Theoretical foundations of Monte Carlo simulation, Markov chains, random walks. Study of phase transitions in the 2D and 3D Ising models as well as in the Landau Ginsburg Model using Monte Carlo simulations. Brownian Dynamics as an example of simulation for the study of stochastic systems.
Objectives:
-Introduce students to the micro-canonical, canonical, and grand-canonical Statistical Ensembles as well as the Maxwell-Boltzmann, Fermi-Dirac, and Bose-Einstein Distribution laws;
-Introduce students to the theoretical foundations of Monte Carlo Simulations;
-Introduce students to the micro-canonical, canonical, and grand-canonical Monte Carlo Simulations in the study of simple systems;
-Introduce Students to Brownian Dynamics in the study of simple stochastic systems;

2020,2021

PHYS431: Monte Carlo Simulations in Statistical Mechanics
(3 credits)
Description: Review of pertinent topics in classical and quantum physics. Gibb's statistical

ensembles, MB, BE, and FD statistics with simple applications to solids. Theoretical foundations of Monte Carlo simulation, Markov chains, random walks. Study of phase transitions in the 2D and 3D Ising models as well as in the Landau Ginsburg Model using Monte Carlo simulations. Brownian Dynamics as an example of simulation for the study of stochastic systems.
Objectives:
-Introduce students to the micro-canonical, canonical, and grand-canonical Statistical Ensembles as well as the Maxwell-Boltzmann, Fermi-Dirac, and Bose-Einstein Distribution laws;
-Introduce students to the theoretical foundations of Monte Carlo Simulations;
-Introduce students to the micro-canonical, canonical, and grand-canonical Monte Carlo Simulations in the study of simple systems;
-Introduce Students to Brownian Dynamics in the study of simple stochastic systems;

2020,2021

PHYS102: General Physics
A continuation of PHYS101. Topics covered include: wave motion and sound; temperature, first and second law of thermodynamics; kinetic theory of gases; Coulomb's law; the electric field; Gauss' law; electric potential; capacitors and dielectrics; D.C. circuits; the magnetic field; Ampere's and Faraday's laws.
This course is for undergraduate students.
Textbook: "Principles of Physics", by Halliday, Resnick and Walker, Tenth Edition, John Wiley & Sons, Inc (2014).

2020,2021

PHYS101: General Physics
The topics covered include particle kinematics and dynamics; conservation of energy and linear momentum; rotational kinematics; rigid body dynamics; conservation of angular momentum; Gravitation; simple harmonic motion; the static and dynamics of fluids.
This course is for undergraduate students.
Textbook: "Principles of Physics", by Halliday, Resnick and Walker, Tenth Edition, John Wiley & Sons, Inc (2014).

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 (PHYS1025Q)
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.

Certificate the completion of courses

- "Communicate With Confidence", American Management Association, New York, 2019
- "Colleage Science Teaching", University of Michigan, Ann Arbor, 2018
- "Teaching Assistant Orientation", University of Connecticut, 2003

Training

College Teaching in Science and Engineering University of Michigan
Ann Arbor,MI Jan-Mar,2018
This is an eight-week short course for training on college teaching in Science and Engineering
The course topic includes:
(1) Trends in STEM Education
(2) Course Design
(3) Science of Learning
(4) Assessment and Feedback
(5) Active and Inquiry-Based Learning
(6) Inclusive Teaching in the STEM Classroom
(7) Group Work and Project Design

All sessions are integrated and build upon one another, leading participants to capstone experiences in practice teaching sessions.
Note: The **certification** *of this training is available on request.*

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).

Undergrad/graduate Advisors
Mentoring Graduate students University of Michigan
Ann Arbor, MI, USA 2016 – 2018
(1) Liangliang Niu: Molecular dynamics simulations of defect aggregation and diffusion in tungsten. (graduated in 2017)
(2) Tao Lu: Hydrogen aggregation and diffusion in metals.
(3) Nanjun Chen: Multiscale modeling the diffusion of fission products in SiC.
(4) Mike Higgins: Plasticity of steels under irradiation;
(5) Ana Cao: Single cascade radiation damage in steels and SiC.
(6) Hai Huang: Molecular dynamics simulation of cascade radiation damage in Nickel and graphene composite.
(7) Chengguang Liu: Molecular dynamics simulation of cascade radiation damage in $MgAl_2O_4$ spinel.
Outcomes: 4+ publications.

Mentoring Graduate students Wuhan University
2015 – 2018
Weihui Wang: Advanced mechanical properties of graphene including friction. (graduated in 2016).
(2) Yuping Yan: Molecular dynamics simulation of graphene mechanics.
Outcomes: 5+ publications.

Mentoring Graduate students Rensselaer Polytechnic Institute
Troy, NY, USA 2012 – 2018
(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. (graduated in 2018)
(4) Binghui Deng: Modeling advanced mechanical properties of 2D materials using molecular dynamics simulations (graduated in 2017).
(5) Jie Hou: Fitting EAM potentials from DFT calculations for radiation damage modeling of Fe-Al-Cr alloys.

Outcomes: 10+ publications.

Mentoring Undergraduate Rensselaer Polytechnic Institute
Troy, NY, USA 2011 – 2015
(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)
(5) 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).
Outcomes: 3 publications. In addition, Ms. Aaron Liu took part in the Siemens Competition in Math, Science and Technology. The related work was published in 2018, as Aaron Liu, Qing Peng*, "A Molecular Dynamics study of the Mechanical Properties of Twisted Bilayer Graphene", Micromachines,(2018), 9,440.

Mentoring Graduate/undergrads students University of Connecticut
Storrs, CT, USA 2011 – 2015
(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).

Volunteer Services(recently)

EGS Judge University of Michigan
Ann Arbor, MI 2017,2018
Judge for Engineering Graduate Symposium, Engineering school of the University of Michigan. Discussed and Judged the presentations in the session of "Chemical Physics" with rate (scores) of 5 posters among about 60 posters in total.

Research mentor for high school scholars University of Michigan
Ann Arbor, MI 2018
Participating in outreach and research mentorship in University of Michigan's Wolverine Pathways Program, which partners with the families, schools, and communities of Detroit, Southfield, and Ypsilanti to provide free, year-round, educational enrichment to middle and high school scholars. Sharing my experience in designing a research question and project.

PUBLICATION LIST

Publication overview

H-index: 29 by Google Scholar — Web of Science, ResearcherID, i10-index: 64,
more details on ResearchGate, Mendeley, Scopus, and ORCID
Total papers: 159; (on February 27, 2021) (IF : Impact Factor, for reference only)

- **151 Peer-reviewed journal papers**
  - mean impact factor: 3.700
  - Total citations: 3124
  - *first-* and *corresponding* authored: 100
- 6 Conference papers (Full length, peer-reviewed)
- 2 Book chapters

Peer−reviewed Journal papers

Subtotal 151 (* denotes corresponding author)

[1] **Q. Peng***,, S. Peng, Q. Cao, "Ultrahigh ballistic resistance of twisted bilayer graphene ", *Crystals*, (2021) **11**, 120. (Impact Factor 2.404)

[2] Z. Sun, J. Zhang, H. Wang, G. Pan, X. Lu, **Q. Peng***,, "Defect, temperature, and strain effects on lattice heat conductivity of egg-tray graphene ", *Modelling and Simulation in Materials Science and Engineering*, (2021) **accepted**, xxx. (Impact Factor 1.874)

[3] **Q. Peng***,, "Performance of SCAN meta-GGA functionals on nonlinear mechanics of Graphene-like g-SiC ", *Crystals*, (2021) **11**, 120. [link] (Impact Factor 2.404)

[4] Y. Bai, J. Liu, P. Ren, W. Guo, T. Wang, W. Chen, X. Liu, **Q. Peng**,, Y. Song, Y. Yang, Y. Li, X. Wen, "Oxygen Adsorption-Induced Morphological Evolution of Hagg Iron Carbide at High Oxygen Chemical Potentials ", *The Journal of Physical Chemistry C*, (2021) **125**, 3055 – 3065 [link] (Impact Factor 4.189)

[5] L. Wang, J. Jin, P. Yang, S. Li, S. Tang, Y. Zong, **Q. Peng***,, "Effect of interfacial bonding on dislocation strengthening in graphene nanosheet reinforced iron composite: a molecular dynamics study ", *Computational Materials Science*, (2021) **191**, 110309. [link] (Impact Factor 2.863)

[6] **Q. Peng***,, B. Deng, M Utz, "Reduced Plastic Dilatancy in Polymer Glasses ", *Macromolecular Theory and Simulations*, (2020) **151**, 109909 [link] (Impact Factor 1.636)

[7] Z. Tian, H. Yan, **Q. Peng***, L. Guo, S. Zhou, C. Ding, P. Li, Q. Luo, " Atomistic Insights into Aluminum Doping Effect on Surface Roughness of Deposited Ultra-thin Silver Films", *Nanomaterials*, (2021) **11**, 158. [link] (Impact Factor 4.324)

[8] H. Huang, X. Tang, K. Xie, **Q. Peng**,, "Enhanced self-healing of irradiation defects near a Ni-graphene interface by damaged graphene: Insights from atomistic modeling ", *Journal of Physics and Chemistry of Solids*, (2021) **151**, 109909. [link] (Impact Factor 3.570)

[9] P. Wang, Q. Cao, H. Wang, S. Liu, Y. Chen, **Q. Peng***,, "CNT-sandwiched copper composites as super thermal conductors for heat management ", *Physica E: Low-dimensional Systems and Nanostructures*, (2021), **114**, 114557. [link] (Impact Factor 3.442)

[10] J. Liu, T. Yang,**Q. Peng***,, Y. Yang, Y. Li, X. Wen, "Theoretical Exploration of the Interaction between Hydrogen and Pyrite-type FeS2 Surfaces ", *Applied Surface Science*, (2021), **537**, 147900 [link] (Impact Factor 6.182)

[11] L. Jiang,**Q. Peng***,, P. Xiu, Y. Yan, Z. Jiao, C. Lu, T. Liu, C. Ye, R. Shu, Y. Liao, Q. Ren, F. Gao, L. Wang, "Elucidating He-H assisted cavity evolution in alpha Cr under multiple ion beam irradiation ", *Scripta Materialia*, (2020), **187**, 291 [link] (Impact Factor 5.079)

[12] Y. Li, R. Li,**Q. Peng***,, S. Ogata, "Reduction of dislocation, mean free path, and migration barriers by high entropy alloy: insights from atomistic study of irradiation damage of CoNiCrFeMn ", *Nanotechnology*, (2020), **published online**, DOI: 10.1088/1361-6528/ab9cf5 [link] (Impact Factor 3.551)

[13] L. Zhang, H. Chen, X. Tao, H. Cai, J. Liu, Y. Ouyang,**Q. Peng**,, Y. Du, "Machine learning reveals the importance of the formation enthalpy and atom-size difference in forming phases of high entropy alloys ", *Materials & Design*, (2020), **193**,108835 [link] (Impact Factor 6.289)

[14] **Q. Peng***, "High-order Nonlinear Mechanical Properties of g-SiC ", *Mechanics of Materials*, (2020), **148**, 103473 [link] (Impact Factor 2.993)

[15] H. Wan, X. Liu, M. Qing, **Q. Peng**, Y. Zhang, S. Liu, H. Wang, X. Wen, Y. Yang, Y. Li, "Surface Structure and Morphology Evolution of Iron Borides under Dynamic Conditions: A Theoretical Study ", *Applied Surface Science*, (2020), **525**, 146462 [link] (Impact Factor 6.182)

[16] H. Gong, Y. He, S. Liu, M. Qing, **Q. Peng***, C. Huo, H. Wang, Y. Yang, X. Wen, "Electronic effects of transition metal dopant Fe(100) and Fe5C2 (100) surfaces for CO activation ", *Catalysis Science and Technology*, (2020), **10**, 2047-2056 [link] (Impact Factor 5.721)

[17] Q. Qin, T. Sun, H. Wang, P. Brault, H. An, X. Lu, **Q. Peng***, "Adsorption and Diffusion of Hydrogen in Carbon Honeycomb ", *Nanomaterials*, (2020), **10**, 344. [link] (Impact Factor 4.324)

[18] Z. Su, S. Wang, C. Lu, **Q. Peng**, "Relationship between the Behavior of Hydrogen and Hydrogen Bubble Nucleation in Vanadium ", *Materials*, (2020), **13**, 322. [link] (Impact Factor 3.057)

[19] H. Yu, G. Huang, **Q. Peng**, L. Chen, H. Pang, X. Qin, P. Qiu, X. Shi, L. Chen, X. Chen, "A combined experiment and first-principles study on lattice dynamics of thermoelectric CuInTe2 ", *Journal of Alloys and Compounds*, (2020), **822**, 153610. [link] (Impact Factor 4.650)

[20] Y. Yang, Q. Cao, S. Lei, S. Liu,**Q. Peng***, "High impact resistance in graphyne ", *RSC Advances*, (2020), **10**, 1697. [link] (Impact Factor 3.119)

========== KFUPM ==========

[21] L. Xie, T. Sun, C. He, J. Deng, H. Yi, X. Yang, Q. Qin,**Q. Peng***, "Enhancement of toughness of SiC through compositing SiC-Al interpenetrating phase composites ", *Nanotechnology*, (2020), **31**, 135706. [link] (Impact Factor 3.551)

[22] M. Xing, A. D. Pathak, S. Sanyal,**Q. Peng**, X. Liu, X. Wen, "Temperature-Dependent Surface Free Energy and the Wulff Shape of Iron and Iron Carbide Nanoparticles: A Molecular Dynamics Study ", *Applied Surface Science*, (2020), **509**, 144859, [link] (Impact Factor 6.182)

[23] **Q. Peng***, "Graphene Mechanics ", *Crystals*, (2019), **9** (12), 636 [link] (Impact Factor 2.404)

[24] P. Wang, Q. Cao, H. Wang, Y. Nie, S. Liu, **Q. Peng***, "Fivefold enhancement of yield and toughness of copper nanowires via coating carbon nanotubes ", *Nanotechnology*, (2020), **31**, 115703 [link] (Impact Factor 3.551)

[25] Q. Cao, S. Zheng, C.P. Wong, S. Liu, **Q. Peng***, "Massively Engineering the Wettability of Titanium by Tuning Nanostructures and Roughness via Laser Ablation ", *The Journal of Physical Chemistry C*, (2019), **123**, 30382-30388 [link] Featured Article on the Cover with cover art (Impact Factor 4.189)

[26] L. Wang, J. Jin, P. Yang, Y. Zong, **Q. Peng***, "Graphene adhesion mechanics on metal surfaces: insights from atomistic study ", *Crystals*, (2019), **9**, 579. [link] (Impact Factor 2.404)

[27] D. Gu, X. Tao, H. Chen, W. Zhu, Y. Ouyang, Y. Du, **Q. Peng***, "Highly Efficient Polarized GeS/MoSe2 Van Der Waals Heterostructure for Water Splitting under Ultraviolet to Near Infrared Light ", *physica status solidi (RRL) - Rapid Research Letters*, (2019), **19**, 1900582 [link] (Impact Factor 2.291)

[28] N. Chen, **Q. Peng**, Z. Jiao, I. van Rooyen, W. F. Skerjanc, F. Gao, "Analytical Bond-order Potential for Silver, Palladium, Ruthenium and Iodine Bulk Diffusion in Silicon Carbide", *Journal of Physics: Condensed Matter*, (2020), **32**, 085702 [link] (Impact Factor 2.707)

[29] T. Shi, **Q. Peng**, Z. Bai, F. Gao, I. Jovanovic, "Proton irradiation of graphene: insights from atomistic modeling ", ***Nanoscale***, (2019), **11**, 20754-20765 [link] (Impact Factor 6.895)

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[128] **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) (Impact Factor 1.224)

[129] **Q. Peng*** , X. Chen, W. Ji and S. De, "Chemically Tuning Mechanics of Graphene by BN", *Advanced Engineering Materials*, **15**, 718–727 (2013). [link] (Impact Factor 2.319)

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[131] **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] (Impact Factor 2.993)

[132] **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] (Impact Factor 3.119)

[133] **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] (Impact Factor 2.485)

[134] **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] (Impact Factor 3.430)

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[136] **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] Highlighed/reported in News: VerticalNews: Zinc Compounds:Advances in Research and Application (Impact Factor 2.863)

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[138] **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] (Impact Factor 2.102)

[139] **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] (Impact Factor 3.430)

[140] **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] (Impact Factor 2.485)

[141] **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] (Impact Factor 2.863)

[142] **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] (Impact Factor 3.570)

[143] **Q. Peng*** and R. E. Cohen, "Origin of Pyroelectricity in LiNbO3". *Physical Review B*, **83**, 220103(R) (2011). [link] (Rapid Communications) (Impact Factor 3.575)

[144] **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) (Impact Factor 5.000)

[145] 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] (Impact Factor 2.863)

[146] 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] (Impact Factor 3.575)

[147] **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] (Impact Factor 1.874)

[148] **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] (Impact Factor 1.874)

[149] **Q. Peng***, X. Zhang, and G. Lu, " Quantum mechanical simulations of nanoindentation of Al thin film", *Computational Materials Science*, **47**, 769 (2010) [link] (Impact Factor 2.863)

[150] **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) (Impact Factor 3.575)

[151] 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] (Impact Factor 2.489)

Conference Proceedings

– *full length, peer-reviewed:* (Subtotal: 6)

[1] N. Chen, **Q. Peng**, Z. Jiao, I. J. van Rooyen, W. Skerjanc, F. Gao, "Fission Product Transport in TRISO Fuel: A Computational Study", Transactions of the American Nuclear Society, (2018), **119**, 407-410. [online]— [Local PDF]

[2] G. Wang, G. R. Liu, **Q. Peng** and S. De, "A micro-macro coupling approach of MD-SPH method for reactive energetic materials", *AIP Conference Proceedings*, **1793**, 05006 (2017). [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: 2)

[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]

PRESENTATIONS

Total 66

Keynote

(Subtotal 3)

[1] "High-order nonlinear mechanical properties of g-SiC", on The 11th International Conference on Computational Methods, Aug 9 - 12, 2020, Virtual Conference

[2] "Mystery of the formation of 100 loops in irradiated iron", "First Regional Virtual Symposium on Physics Advances", Jun 28-29, 2020, University of Bahrain, Bahrain.

[3] "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 World Chemistry Conference and Exhibition, Sep 04 - 06, 2017, Rome, Italy on "7th International Advances in Applied Physics and Materials Science Congress" (APMAS2017) April 22, 2017 in Oludeniz, Fethiye, TURKEY.

Invited *Conference* Talks

(Subtotal 9)

[1] "Enhancement of toughness of SiC through compositing SiC-Al interpenetrating phase composite", "The 1st KFUPM-Saudi Aramco Joint Technical Exchange Meeting on Advances in Nanometallic Materials", Feb 26, 2020, KFUPM, Saudi Arabic.

[2] "Silver bulk diffusion in 3C-SiC: insensitive to charge status", "The 2018 Computer Simulation of Radiation Effects in Solids (COSIRES2018)", June 18-22, 2018, Shanghai University, Shanghai, China.

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

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

[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] "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.

[7] "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

[8] "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.

[9] "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

Conferences

(Subtotal 28)

[1] "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.

[2] "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.

[3] "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.

[4] "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

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

[6] "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

[7] "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

[8] "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, 2014, 15th International Detonation Symposium (IDS), San Francisco, CA.

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

[10] "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.

[11] "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.

[12] "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.

[13] "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

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

[15] "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

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

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

[18] "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.

[19] "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.

[20] "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.

[21] "A QCDFT Study of Hydrogen embrittlement at Crack Tip", Qing Peng, Mar 22, 2011, APS March Meeting, Dallas, TX. [link]

[22] "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

[23] "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

[24] "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.

[25] "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]

[26] "First Principle Based Computation of Pyroelectricity in LiNbO3", Q. Peng, R. E. Cohen, March 18,2010, APS March Meeting, Portland, OR [link]

[27] "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 [link]

[28] "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

Invited Seminar Talks

Subtotal 26

[1] "Nanophysics", Qing Peng, Oct 25, 2020. Physics department, King Fahd University of Petroleum and Minerals, Saudi Arabia

[2] "Mystery of the Formation of $< 100 >$ Loops in Irradiated Iron", Qing Peng, Sept 9, 2020. Department of Scientific Computing, Florida State University.

[3] "QCDFT insights into the hydrogen embrittlement", Qing Peng, Sept 7, 2020. Physics department, King Fahd University of Petroleum and Minerals, Saudi Arabia.

[4] "Mystery of the Formation of $< 100 >$ Loops in Irradiated Iron", Qing Peng, Feb 11, 2020. Physics department, King Fahd University of Petroleum and Minerals, Saudi Arabia.

[5] "Mystery of the Formation of $< 100 >$ Loops in Irradiated Iron", Qing Peng, Nov 16, 2018. Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, USA.

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

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

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

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

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

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

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

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

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

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

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

[17] "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]

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

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

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

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

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

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

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

[25] "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]

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