Liang Qi

Room 211, 3231 Walnut Street
Philadelphia, PA 19104
(215)-573-8440
liangqi@seas.upenn.edu

Education

University of Pennsylvania — Philadelphia, PA
Department of Materials Science and Engineering (2007-2009) — Ph.D.

Ohio State University — Columbus, OH
Department of Materials Science and Engineering (2003-2007) — M.S.

Tsinghua University — Beijing, P.R.C.
Department of Materials Science and Engineering (1999-2003) — B.E.

Research Interests

Theoretical and computational materials science.

Research Experience

Postdoctoral Researcher, Supervisor: Prof. Ju Li — 2009.9∼
Materials theory group, University of Pennsylvania

Graduate Research Assistant, Supervisor: Prof. Ju Li — 2003.9∼2009.8
Materials theory group, Ohio State University (2003.9∼2007.9) and University of Pennsylvania
- Multiscale modeling of electrocatalysis in PEM fuel cell.
- Theoretical study of graphene.
- Density functional theory study of DeNOx catalysts.
- Atomic modeling of mechanical properties of materials.
- Kinetic Monte Carlo simulation on titania nanofiber formation.

Research Assistant, Supervisor: Prof. Changan Wang — 2003.1∼2003.7
State Key Laboratory of New Ceramics and Fine Processing, Tsinghua University
- Synthesis of pure ternary carbide Ti_3AlC_2 powder.

Research Assistant, Supervisor: Prof. Heping Zhou — 2002.1∼2002.12
State Key Laboratory of New Ceramics and Fine Processing, Tsinghua University
- Low-temperature sintering of aluminum nitride ceramics.

Publications

5. J. Feng, L. Qi, J-Y. Huang and J. Li, Geometric and Electronic Structures of Graphene Bilayer Edges, accepted by *Phys. Rev. B*.

4. J-Y. Huang, D. Feng, B. I. Yakobson, P. Lu, L. Qi, and J. Li, "In-situ observation of graphene sublimation and multi-layer edge reconstructions: genesis of interconnected carbon nanostructures," *Proc. Natl. Acad. Sci.* **106** (2009) 10103-10108.

3. X-F. Qian, J. Li, L. Qi, C-Z. Wang, T-L. Chan, Y-X. Yao, K-M. Ho and S. Yip, "Quasiatomic orbitals for *ab initio* tight-binding analysis," *Phys. Rev. B* **78** (2008) 245112.

2. L. Qi, X-F. Qian and J. Li, "Near-neutrality of oxygen molecule adsorbed on Pt(111) surface," *Phys. Rev. Lett.* **101** (2008) 146101.

1. L. Qi, J-G. Yu and J. Li, "Coverage dependence and hydroperoxyl-mediated pathway of catalytic water formation on Pt (111) surface," *J. Chem. Phys.* **125** (2006) 054701.

Presentations

7. "First-principles studies of long-period structures (LPS) in Mg alloys," *10th U.S. National Congress for Computational Mechanics*, Columbus, OH, July, 2009.

6. "Electronic structure of intermediates in oxygen reduction reaction on Pt electrode," *American Chemical Society, 237nd National Meeting & Exposition*, Salt Lake City, UT, Mar 25, 2009.

5. "First Principles studies of Pt electrode in PEM fuel cell," *37th Seminar on Mechanical Science and Bioengineering, Graduate School of Engineering Science, Osaka University*, Osaka, Japan, October 3, 2008.

4. 'First-principles studies of surface oxide formation on Pt electrode," *American Chemical Society, 236nd National Meeting & Exposition*, Philadelphia, PA, Aug 20, 2008.

3. "Reaction path of water formation on Pt(111) surface under UHV condition and alloying effects," *American Chemical Society, 232nd National Meeting & Exposition*, San Francisco, CA USA, Sep 13, 2006.

2. "DFT modeling of nanoclusters for PEM fuel cell," *2005 Materials Research Society, 2005 Fall Meeting*, Boston, MA, Nov 29, 2005.

1. "Hydronium on Pt (111) surface and their roles in O_2 reduction," *American Chemical Society, 230nd National Meeting & Exposition*, Washington, D. C., Aug. 29, 2005.

Miscellaneous

Visiting Researcher
Fundamental Technology Research Center, Honda R&D Co., Ltd., Wako-shi, Saitama, Japan.
Project:"Theoretical study of long-period structures in Mg alloys" 2008.9∼2008.10

Builder of

16-CPU 64-bit high-performance parallel computing PC cluster at OSU 2006.10
14-CPU Gigabit high-performance parallel computing PC cluster at OSU 2003.12