Fei Zhou (周非)

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Education

- PhD in Physics, Massachusetts Institute of Technology, Cambridge, MA *August 2006*
- BS in Physics, University of Science and Technology of China, Hefei, China *June 2001*

Research Interests

My primary research interests are in theoretical and computational studies of solid state materials for energy applications:

- Transition metal oxides as cathode of primary as well as rechargeable lithium-ion battery;
- Supercapacitor
- actinide compounds for nuclear fuel;
- designing of hydrogen storage materials;
- effects of electron correlation and electronic entropy in the kinetics and thermodynamics of transition metal, lanthanide and actinide oxides at both the bulk and nano-scale.

I am also interested in spintronics and coarse-grained models for protein interactions and the bio-nano interface.

Research Experience

Postdoc, Dept. Materials Science and Engineering, UCLA, Los Angeles, CA *August 2008 - present*
Advisor: Vidvuds Ozolins
Development of an electronic structure method based on LDA+U that removes the aspherical self-interaction errors of conventional methods. Other work with collaborators includes hydrogen storage materials, materials for spintronics applications and computational characterization of supercapacitor performance.

Postdoc, Dept. Materials Science and Engineering, MIT, Cambridge, MA *Sept. 2006 - July 2008*
Advisor: Gerbrand Ceder
Worked on the thermodynamics of transition metal oxides as battery cathode, with focus the bulk, interface and surface properties of Li_xFePO_4. Investigating the effects of electronic entropy of localized electrons and holes. First-principles data-mining and high-throughput approaches to study general oxides for energy applications. Charge, orbital and electron-phonon interactions and the Verwey transition in Fe_3O_4.

Graduate research assistant, Department of Physics, MIT, Cambridge, MA *Sept. 2001 - August 2006*
Advisor: Gerbrand Ceder and John Joannopoulos
Explored with computational methods the electron correlation effects in transition metal oxides (TMO), as well as the energetics of proteins and nanotube-protein interface. The former results showed that the correlation effects of transition metal d-electrons are essential for accurate theoretical characterization of TMO properties, including band gap, magnetization, lattice parameters, reaction energy and thermal stability.

Publications & Talks

Journal articles

1. R. Malik, F. Zhou, and G. Ceder, Phase Diagram and Electrochemical Properties of Mixed Olivines from First Principles, *Physical Review B* **79**, 214201 (2009)
2. L. Wang, F. Zhou, and G. Ceder, Ab-initio Study of the Surface Properties and Nano-scale Effects of $LiMnPO_4$, *Electrochemical and Solid-State Letters* **11**, A94 (2008)
3. L. Wang, F. Zhou, Y. S. Meng, and G. Ceder, First-principles study of surface properties of $LiFePO_4$: Surface energy, structure, Wulff shape, and surface redox potential, *Physical Review B* **76**, 165435 (2007)
4. F. Zhou, T. Maxisch, and G. Ceder, Configurational electronic entropy and the phase diagram of mixed-valence oxides: The case of Li_xFePO_4, *Physical Review Letters* **97**, 155704 (2006)
5. G. Grigoryan , F. Zhou , S. Lustig , G. Ceder , D. Morgan and A. E. Keating, Ultra-fast Evaluation of Protein Conformational Energies Directly from Sequence, *PLoS Computational Biology* **2**, e63 (2006)
6. T. Maxisch, F. Zhou, and G. Ceder, Ab initio study of the migration of small polarons in olivine Li_xFePO_4 and their association with lithium ions and vacancies, *Physical Review B* **73**, 1 (2006)
7. F. Zhou, G. Grigoryan, S. R. Lustig, A. E. Keating, G. Ceder, and D. Morgan, Coarse-graining protein energetics in sequence variables, *Physical Review Letters* **95**, 148103 (2005)
8. F. Zhou, M. Cococcioni, C. A. Marianetti, D. Morgan, and G. Ceder, First-principles prediction of redox potentials in transition-metal compounds with LDA +U, *Physical Review B* **70**, 235121 (2004)
9. F. Zhou, M. Cococcioni, K. Kang, and G. CedeR. The Li intercalation potential of $LiMPO_4$ and $LiMSiO_4$ olivines with M = Fe, Mn, Co, Ni, Electrochemistry Communications **6**, 1144 (2004)
10. F. Zhou, K. Kang, T. Maxisch, G. Ceder, and D. Morgan. The electronic structure and band gap of $LiFePO_4$ and $LiMnPO_4$. *Solid State Communications* **132**, 181 (2004)
11. F. Zhou, C. A. Marianetti, M. Cococcioni, D. Morgan, and G. Ceder, Phase Separation in Li_xFePO_4 Induced by Correlation Effects, *Physical Review B* **69**, 201101(R) (2004)
12. F. Zhou, W. G. Ma, Y. Jiang, X. Q. Li and L. H. Wan, Loop induced $W^{\pm}H^{\mp}$ associated production via photon-photon collisions in the two-Higgs-doublet model and the minimal supersymmetric standard model, *Physical Review D* **64**, 055005 (2001)
13. F. Zhou, W. G. Ma, Y. Jiang, L. Han and L. H. Wan, Improved calculation of $W^{\pm}H^{\mp}$ associated production via gluon-gluon fusion at the CERN LHC, *Physical Review D* **63**, 015002 (2000)
14. F. Zhou, W. G. Ma, Y. Jiang and L. Han, Pair production of neutralinos via photon-photon collisions, *Physical Review D* **62**, 115006 (2000)

Preprint

1. F. Zhou and V. Ozolins, Impact of cation ordering in the electronic structure of $La_{2-2x}Sr_{1+2x}Mn_2O_7$, in preparation
2. E.H. Majzoub, F. Zhou and V. Ozolins, Structure Optimization Using Wang-Landau Monte Carlo: Application to Lennard-Jones Clusters, in preparation
3. F. Zhou and V. Ozolins, Obtaining the correct orbital ground state of PrO_2 using a nonspherical self-interaction corrected LDA+U method, in preparation
4. F. Zhou and G. Ceder, First-principles determined charge and orbital interactions in Fe_3O_4, submitted
5. F. Zhou and G. Ceder, First-principles Study of the $FePO_4$/$LiFePO_4$ Interface, in preparation

Invited and Contributed Presentations

1. "First principles studies of Li_xFePO_4", Univ. of Southern California, April 3, 2009
2. "Obtaining the correct orbital ground state of f-electron systems using an aspherical self-interaction corrected LDA+U", APS March Meeting, Pittsburgh, March 18, 2009
3. "First-principles determined charge and orbital interactions in Fe_3O_4", APS March Meeting, Pittsburgh, March 18, 2009
4. "First-principles Study of the $FePO_4$/$LiFePO_4$ Interface and Transport Properties", MRS Spring Meeting, San Francisco, CA, March 26, 2008
5. "Configurational Electronic Entropy and the Phase Diagram of Mixed-Valence Oxides: The Cases of Li_xFePO_4 and Fe_3O_4", APS March Meeting, New Orleans, March 14, 2008
6. "Surface and particle-size effects on the miscibility gap of LixFePO4 from first-principles calculations", Materials Research Society Fall Meeting, Boston, MA, November 30, 2007
7. Lei Wang, Fei Zhou, Ying S. Meng, and G.erbrand Ceder,"First-principles study of surface properties of $LiFePO_4$: Surface energy, structure, Wulff shape, and surface redox potential", Solid State Ionics meeting-16, Shanghai, July 2007
8. Dane Morgan, Fei Zhou, Gerbrand Ceder, Gevorg Grigoryan, Amy Keating, Steve Lustig, "Cluster Expansion for Protein Design", MS&T meeting, Detroit, April 16, 2007
9. Gerbrand Ceder, Fei Zhou, Thomas Maxisch, Lei Wang,"Transport and Phase Stability in LiFePO4", Electrochemical Society Meeting, Cancun 2006
10. "The Unusual Role of Electronic Entropy in the Phase Diagram of Li_xFePO_4", Institute of Physics, Chinese Academy of Sciences, Beijing, China, August 2006
11. "The Unusual Role of Electronic Entropy in the Phase Diagram of Li_xFePO_4", MRS Fall meeting, Boston MA, Nov. 28, 2006
12. "Coarse-graining protein energetics in sequence variables", APS March meeting, Baltimore, MD, Mar. 13, 2006
13. "Electron-correlation induced phase separation in Li_xFePO_4", APS March meeting, Baltimore, MD, Mar. 13, 2006
14. "First principles study of the phase diagram of Li_xFePO_4", MRS Fall meeting, Boston MA, Nov. 28, 2005
15. "Design of nanotube-binding peptides assisted by cluster expansion", DuPont-MIT Alliance Symposium, Cambridge, MA, Sept. 20, 2005
16. "Coarse graining protein energetics with cluster expansion", Singapore-MIT Alliance Symposium, Singapore, Jan. 19, 2005
17. "A DFT+U study of electron correlation effects on total energy calculation of transition-metal compounds", MRS Fall meeting, Boston MA, Dec 2, 2004
18. "Coarse graining protein energetics with cluster expansion", Dupont-MIT Alliance Symposium, Cambridge, MA, Oct 13, 2004

Teaching Experience

MIT Department of Materials Science and Engineering, Cambridge, MA *March, 2008*
Gave a lecture on the introduction of density functional theory to the class of 3.320, a graduate-level course on materials modeling

MIT Department of Physics, Cambridge, MA
Physics 8.01x. Recitation instructor and laboratory teaching assistant *Sept. 2002 – Dec. 2002*

Gave recitation sessions to undergraduate students in the introductory physics class. Supervised and instructed students with take-home experiments. Grading of experiments and exams.

MIT Project Interphase. Lecture instructor *June 2002 – August 2002*
Prepared teaching materials including slides, problem sets and exams for freshman students in the physics class. Gave lectures.

Awards

William M. Layson Presidential Fellowship of MIT (2001), Second Class Prize for the 7th National Challenge Cup of China (2001), First Class Award for Undergraduate Thesis of USTC (2001)

Activities

Referee for Solid State Ionics. Member, American Physical Society. Member, Materials Research Society. Interests include swimming, boating, reading, history.

Status

H1-B Visa. Chinese citizen. Married.

References

- Professor Vidvuds Ozolins
  Dept. Materials Science and Engineering, UCLA
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- Professor Gerbrand Ceder
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- Professor John Joannopoulos
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