

# 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

- Theoretical and computational understanding of strongly correlated materials, specifically transition metal oxides and lanthanide and actinide compounds
- Modeling of oxide materials for electrochemistry applications, including lithium-ion battery cathode and supercapacitor
- Nanoparticles for energy applications, e.g. battery and hydrogen storage
- Other interests: spintronics, coarse-grained protein interaction models and the bio-nano interface.

## Research Experience

Postdoc, Dept. Materials Science & Engineering, UCLA, Los Angeles, CA *Aug. 2008 - Aug. 2009*  
Research Engineer, *Sept. 2009 - present*

Advisor: Vidvuds Ozolins

Development of an electronic structure method 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 & Engineering, MIT, Cambridge, MA *Sept. 2006 - July 2008*

Advisor: Gerbrand Ceder

Thermodynamics of transition metal oxides as battery cathode, with focus the bulk, interface and surface properties of  $\text{Li}_x\text{FePO}_4$ . First-principles data-mining and high-throughput approaches to battery design. Charge and orbital interactions and the Verwey transition in  $\text{Fe}_3\text{O}_4$ .

Graduate researcher, Department of Physics, MIT, Cambridge, MA *Sept. 2001 - August 2006*

Advisors: 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  $\text{LiMnPO}_4$ ", *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  $\text{LiFePO}_4$ : 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  $\text{Li}_x\text{FePO}_4$ ", *Physical Review Letters* **97**, 155704 (2006)
5. G. Grigoryan, F. Zhou, S.R. 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  $\text{Li}_x\text{FePO}_4$  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  $\text{LiMPO}_4$  and  $\text{LiMSiO}_4$  olivines with  $M = \text{Fe, Mn, Co, Ni}$ ", *Electrochemistry Communications* **6**, 1144 (2004)
10. F. Zhou, K. Kang, T. Maxisch, G. Ceder, and D. Morgan, "The electronic structure and band gap of  $\text{LiFePO}_4$  and  $\text{LiMnPO}_4$ ", *Solid State Communications* **132**, 181 (2004)
11. F. Zhou, C. A. Marianetti, M. Cococcioni, D. Morgan, and G. Ceder, "Phase Separation in  $\text{Li}_x\text{FePO}_4$  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, "Obtaining the correct orbital ground state of  $\text{PrO}_2$  using a nonspherical self-interaction corrected LDA+ $U$  method", submitted
2. F. Zhou and G. Ceder, "First-principles determined charge and orbital interactions in  $\text{Fe}_3\text{O}_4$ ", submitted
3. F. Zhou and V. Ozolins, "The electronic structure of  $\text{UO}_2$ : a first-principles probe of the ground and excited states", in preparation

4. F. Zhou, L. Wang and G. Ceder, "First-principles Study of the  $\text{FePO}_4/\text{LiFePO}_4$  Interface", in preparation
5. E.H. Majzoub, F. Zhou and V. Ozolins, "Structure Optimization Using Wang-Landau Monte Carlo: Application to Lennard-Jones Clusters", in preparation

#### Invited and Contributed Presentations

1. "Electronic structure of  $\text{UO}_2$ ", UC Davis, June 5, 2009
2. "First principles studies of  $\text{Li}_x\text{FePO}_4$ ", Univ. of Southern California, April 3, 2009
3. "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
4. "First-principles determined charge and orbital interactions in  $\text{Fe}_3\text{O}_4$ ", APS March Meeting, Pittsburgh, March 18, 2009
5. "Obtaining the correct orbital ground state of f-electron systems using a non-spherical self-interaction corrected LDA+ $U$ ", UC Davis, Feb. 18, 2009
6. "First-principles Study of the  $\text{FePO}_4/\text{LiFePO}_4$  Interface and Transport Properties", MRS Spring Meeting, San Francisco, CA, March 26, 2008
7. "Configurational Electronic Entropy and the Phase Diagram of Mixed-Valence Oxides: The Cases of  $\text{Li}_x\text{FePO}_4$  and  $\text{Fe}_3\text{O}_4$ ", APS March Meeting, New Orleans, March 14, 2008
8. "Surface and particle-size effects on the miscibility gap of  $\text{Li}_x\text{FePO}_4$  from first-principles calculations", Materials Research Society Fall Meeting, Boston, MA, November 30, 2007
9. "The Unusual Role of Electronic Entropy in the Phase Diagram of  $\text{Li}_x\text{FePO}_4$ ", Institute of Physics, Chinese Academy of Sciences, Beijing, China, August 2006
10. "The Unusual Role of Electronic Entropy in the Phase Diagram of  $\text{Li}_x\text{FePO}_4$ ", MRS Fall meeting, Boston MA, Nov. 28, 2006
11. "Coarse-graining protein energetics in sequence variables", APS March meeting, Baltimore, MD, Mar. 13, 2006
12. "Electron-correlation induced phase separation in  $\text{Li}_x\text{FePO}_4$ ", APS March meeting, Baltimore, MD, Mar. 13, 2006
13. "First principles study of the phase diagram of  $\text{Li}_x\text{FePO}_4$ ", MRS Fall meeting, Boston MA, Nov. 28, 2005
14. "Design of nanotube-binding peptides assisted by cluster expansion", DuPont-MIT Alliance Symposium, Cambridge, MA, Sept 20, 2005
15. "Coarse graining protein energetics with cluster expansion", Singapore-MIT Alliance Symposium, Singapore, Jan 19, 2005
16. "A DFT+ $U$  study of electron correlation effects on total energy calculation of transition-metal compounds", MRS Fall meeting, Boston MA, Dec 2, 2004
17. "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 *Sept. 2002 – Dec. 2002*  
Physics 8.01x. Recitation instructor and laboratory teaching assistant. 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

DOE travel award (2006), 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

Chinese citizen. Married.

## References

- Professor Vidvuds Ozolins  
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- Professor Gerbrand Ceder  
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