

Curriculum Vita

Lizhi Ouyang

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Education

- M. S. Computer Science, University of Missouri-Kansas City, 2001
- Ph. D. Physics/Chemistry, University of Missouri-Kansas City, 2000
- M. S. Physics, University of Missouri-Kansas City, 1997
- B. S. Chemical Physics, University of Science & Technology of China, 1993

Appointments

- Assistant Research Professor, 2004-current UMKC
- Lecturer, 2003 UMKC
- Postdoc research associate, 2000-2004 UMKC
- Computational Lab Manager, 1998-current, UMKC

Grants and Awards

- Principle Investigator,
“*First principles calculations of X-ray Absorption Near Edge Structure of Vitamin B12 and its derivatives*”
Alliance Allocations Board Awards, NCSA Xeon Linux Supercluster, 10000 PSU
- Co-principle Investigator,
“*Multi-scale Computational Studies of Interfacial Properties of Collagen/Apatite*”
NIH/NIBIB, pending

Honors and Awards

- Chancellor's Interdisciplinary Ph.D. Fellowship 1998-1999
- Guanghua Award at USTC 1994
- Yilida Award at USTC 1993
- USTC team member in Mathematical Contest in Modeling 1991

Membership

- Sigma Xi
- American Physics Society
- American Association for the Advancement of Science
- American Ceramic Society

Dissertation and Thesis

- Ouyang, Lizhi (2000). *Parallel Computing and First-Principles Calculations: Applications to Complex Ceramics and Vitamin B₁₂*
- Ouyang, Lizhi (1997). A New Approach to Construct Large Periodic Continuous Random Network Model

Funded Research Projects

- “Theoretical Studies on the Electronic Structures and Properties of Complex Ceramic Crystals and Novel Materials” (Continuous funding from the Department of Energy: \$446,306 [07/96-06/99]; \$471,017 [07/99-06/02]; \$487,322 [07/02-06/05])
- “Quantum Structure and Micro-mechanical Response of Ceramic Grain Boundaries” (Jointly Funded by NEDO (Japan) with I.Tanaka, G. Pezzotti, H.J. Kleebe, D. Clarke: Total \$600,000, UMKC \$54,000 [08/00-07/03])
- “Nanometer Scale Induced Structure between Amorphous Layers and Crystalline Materials” (Joint EU/US Program funded by National Science Foundation: US total \$2,103,862 UMKC \$ 245,211 [06/01-08/05]; continuous proposal pending)

Teaching Experiences

- | | |
|---------------------------------------|--------------|
| • Courses taught: | Credit hours |
| General Physics II: Electromagnetism, | 3.0 |
| General Physics Lab I, | 1.0 |
| General Physics Lab II, | 1.0 |

Publications

1. **Lizhi Ouyang**, P. Rulis and W.Y. Ching, “*Electric Structure and Bondings in Hydroxocobalamin*”, (invited paper, Spectrochimica Acta A)
2. **Lizhi Ouyang**, W.Y. Ching, “*Predicting a new high density SiO₂ phase with high dielectric constant*”, submitted, Appl. Phys. Lett..
3. Paul Rulis, Jun Chen, **Lizhi Ouyang**, W.Y. Ching, Xiaotao Su and Stephen H. Garofalini “*Electronic structure and bonding of intergranular glassy films (IGF) in polycrystalline Si₃N₄: Ab-initio studies and classical MD simulations*”, submitted, Phys. Rev. B
4. Jun Chen, Yong-Nian Xu, Paul Rulis, **Lizhi Ouyang**, W.Y. Ching “*Ab-initio tensor experiments on Y-doped $\Sigma=3$ grain boundary in α -Al₂O₃*”, Accepted, Acta Materialia.
5. Paul Rulis, **Lizhi Ouyang**, W.Y. Ching “*Electronic Structure and Bonding in Calcium Apatite Crystals: Hydroxyapatite, Fluoroapatite, Chlorapatite and Bromapatite*”, Phys. Rev. B 70, 155104, 2004.
6. S. Leitch, A. Moewes, **Lizhi Ouyang**, W. Y. Ching, and T. Sekine, “*Properties of non-equivalent sites and band gap of spinel-phase silicon nitride.*” J. Phys.: Condens. Matter 16 6469, 2004
7. W.Y. Ching, **Lizhi Ouyang**, Hongzhi Yao, Y.-N. Xu. “*Electronic structure and bonding in the Y-Si-O-N quaternary crystals*” Phys. Rev. B 70, 045103, 2004
8. **Lizhi Ouyang**, W.Y. Ching “*Electronic Structure and Dielectric Properties of Zr Silicate*” J. Appl.Phys. 95, 7918, 2004

9. **Lizhi Ouyang**, Paul, Rulis, W.Y. Ching, Giorgio Nardin and Lucio Randaccio, "Electronic Structure and Bonding in Adenosylcobalamin" *Inorganic chemistry* 43, 1235, 2004
10. **Lizhi Ouyang**, Hongzhi Yao, Scott Richey, Yong-Nian Xu and W.Y. Ching, "On the Crystal Structure and Properties of $YSiO_2N$ " *Phys. Rev. B.*, March 1, 2004
11. **Lizhi Ouyang**, D.M. Zhu, "Simulation of the Effect of Interstitials to Shear Modulus and Local Vibration Modes in Crystals" (AIP Conf. Proc. "SLOW DYNAMICS IN COMPLEX SYSTEMS", 2003)
12. W.Y. Ching, Yong-Nian Xu and **Lizhi Ouyang**. "Electronic structure and bonding in crystalline $Y_{10}[SiO_4]_6N_2$ ", *J. Amer. Ceramic Soc.* August 2003
13. W.Y. Ching, **Lizhi Ouyang**, and Yong-Nian Xu "Electronic and optical properties of Y_2SiO_5 and $Y_2Si_2O_7$ with comparisons to α - SiO_2 and Y_2O_3 ", *Phys. Rev. B* 67, 245108, 2003
14. W.Y. Ching, Y.-N. Xu, **Lizhi Ouyang**, W. Wong-Ng "Comparative study of the electronic structure of ternary superconductors $MoRuP$ and $ZrRuP$ in the orthorhombic and hexagonal phases", *J. Appl. Phys.* 93 (10): 8209, 2003
15. E.Z. Kurmaev, A. Moewes, M. Bach, M. Neumann, **Lizhi Ouyang**, Lucio Randaccio, Paul Rulis and W.Y. Ching "The electronic structure and chemical bonding of Vitamin B12", *Euro. Phys. Lett.* 62 (4) 582, 2003.
16. **Lizhi Ouyang**, L. Randaccio, P. Rulis, E. Kurmaev, A. Moewes, and W. Y. Ching "Electronic structure and Bonding in Vitamin B₁₂ Cynocobalamin", *J. Mol. Struct. (TheoChem)* 622, 221 (2003)
17. W.Y. Ching, Y.N Xu, and **Lizhi Ouyang** "Electronic and Dielectric Properties of Insulating Zr_3N_4 " *Phys. Rev. B* 66, 235106 (2002)
18. **Lizhi Ouyang**, W. Y. Ching "Electronic Structure and Bonding in the spinel phase $SiAlON$ " *Appl. Phys. Lett.* 81, 229 (2002)
19. **Lizhi Ouyang**, Yong-Nian Xu, W.Y. Ching "Electronic Structure of ZrW_2O_8 ", *Phys. Rev. B* 65, 113110(2002)
20. W.Y. Ching, Shang-di Mo, **Lizhi Ouyang**, Paul Rulis, Isao Tanaka, and Masato Yoshiya "Theoretical Prediction of the Structure and Properties of Cubic Spinel Nitrides", *J. Am. Ceram. Soc.* 85, 75 (2002)
21. W.Y.Ching, Shang-di Mo, **Lizhi Ouyang**, "Electronic and optical properties of cubic phase of c - Si_3N_4 , c - Ge_3N , C - $SiGe_2N_4$, and C - $GeSi_2N_4$ ", *Phys. Rev. B.* 63, 254110 (2001).
22. **Lizhi Ouyang** and W.Y. Ching, "Geometry Optimization and Ground State Properties of Complex Ceramic Oxides", *J. Am. Ceram. Soc.* 84, 891(2001)
23. W.Y. Ching, Shang-di Mo, **Lizhi Ouyang**, IsaoTanaka, and MasatoYoshiya, "Prediction of the new spinel phase of Ti_3N_4 and $SiTi_2N_4$ and the metal-insulator transition", *Phys. Rev. B.* 61, 10609 (2000).
24. W.Y. Ching, Shang-di Mo, **Lizhi Ouyang** and Yong-Nian Xu, "Recent Progress in the Electronic Structure Theory of Complex Ceramics" *Grain Boundary Engineering in Ceramics*, *Ceramic Transaction*, 118, 25, Proceedings of Workshop on JFCC 2000, Neqoya, Japan (2000)
25. W.Y. Ching, **Lizhi Ouyang**, and J.D. Gale, "Full ab initio geometry optimization of all known crystalline phases of Si_3N_4 ", *Phys. Rev. B.* 61, 8696 (2000).
26. Shang-Di Mo, **Lizhi Ouyang**, W.Y. Ching, Isao Tanaka, Yukinori Koyama, and Ralf Riedel, "Interesting Physical Properties of the New Spinel Phase of Si_3N_4 and C_3N_4 ", *Phys. Rev. Lett.* 83, 5046 (1999).

27. M.-Z. Huang, **Lizhi Ouyang**, and W. Y. Ching, "*Electron and phonon states in an ideal continuous random network model of α -SiO₂ glass*", Phys. Rev. B. **59**, 3540 (1999).
28. **Lizhi Ouyang**, and W. Y. Ching, "*Systematic approach to generate near-perfect periodic continuous random network models: application to amorphous Si₃N₄*", Phys. Rev. B: Condens. Matter **54**, R15594 (1996).
29. Houwen Xin, Lingfa Yang, and **Lizhi Ouyang**, "*Calculation of the orientational phase transition temperature in solid C₆₀*", Chin. Phys. Lett. **12**, 473 (1995).
30. Lingfa Yang, **Lizhi Ouyang** and Houwen Xin, "*Theoretical study of orientational transition in solid C₆₀*", Huaxue Wuli Xuebao **8**, 320 (1995).
31. Hou-Wen Xin, Ling-Fa Yang and **Lizhi Ouyang**, "*Theoretical studies of orientational phase transitions in solid C₆₀*", Huaxue Xuebao **52**, 990 (1994).

Cover page publications

- W.Y. Ching, Shang-di Mo, Lizhi Ouyang, Paul Rulis, Isao Tanaka, and Masato Yoshiya "*Theoretical Prediction of the Structure and Properties of Cubic Spinel Nitrides*", J. Am. Ceram. Soc. **85**, 75 (2002) [Title diagram prepared by Lizhi Ouyang]

Presentations and Workshops

- Invited Talk
 1. Lizhi Ouyang, "*Electronic Structures and Bonding in Complex Biomolecules*", APS March meeting, Los Angeles, 2005
 2. Lizhi Ouyang, "*Electronic Structures and Dielectric Properties of Gate material (ZrO₂)_x(SiO₂)_{1-x}*" Dept. of Phys., University of Missouri-Kansas City, 2003
 3. Lizhi Ouyang, "*First principles calculations of complex ceramics and biomolecules*", Los Alamos National Laboratory, NM, Nov. 19 (2001)
- Selected Presentations
 1. Lizhi Ouyang, W.Y. Ching, "*Electronic Structures and Dielectric Properties of Gate material (ZrO₂)_x(SiO₂)_{1-x}*" NANOAM workshop, Boston (2003)
 2. Lizhi Ouyang, W.Y. Ching, "*Structural modeling of composite materials: crystalline Si embedded in amorphous SiO₂*", March meeting, Am. Phys. Soc. Indianapolis (2002)
 3. Paul Rulis, W.Y. Ching, Lizhi Ouyang, "*Electronic Structure and Bonding of Fluoroapatite and Hydroxylapatite*", March meeting, Am. Phys. Soc., Indianapolis(2002)
 4. Lizhi Ouyang, W.Y. Ching, "*Electronic structures of cubic and orthorhombic phase of ZrW₂O₈*", March meeting, Am. Phys. Soc., Seattle (2001)
 5. Lizhi Ouyang, W.Y. Ching, "*Full geometry optimization of complex ceramic crystals by the method of finite-difference in ab-initio total energy*" The American Ceramic Society's 102nd Annual Meeting and Exposition, St. Louis, April 30-May 3, 2000
 6. Lizhi Ouyang, W.Y. Ching, "*Electronic structures of cubic and orthorhombic phase of ZrW₂O₈*", Am. Ceram. Soc., Minneapolis (1998)
 7. Lizhi Ouyang, W.Y. Ching, "*Systematic Construction of Large Periodic Structural Models for Covalent glasses and Interfaces*", March meeting of Am. Phys. Soc., Kansas city, March, 17-21, (1997)

8. Lizhi Ouyang, W.Y. Ching, "Construction of Large Periodic Models for Amorphous Si_3N_4 ", 98th Annual Meeting of American Ceramic Society, Indianapolis, IN, Apr. 14-17, (1996)
- Poster
 1. Lizhi Ouyang, P.Rulis, and W.Y. Ching, "Computational Studies of Apatite Crystals and Surfaces", Goldon Research Conference on Interface in chemistry, Kimball Union Academy, NH, Aug 17-21 (2004)
 2. Lizhi Ouyang, W.Y. Ching, L. Randaccio, "Electronic Structure of B12 coenzyme", DCOMP 2001, Cambridge (20001)
 3. Lizhi Ouyang, W.Y. Ching, "A Systematic Method for Modeling the Structures of Covalent Glasses and Their Interfaces", Golden Research Conference on Solid State Studies in Ceramics, Kimball Union Academy, NH, Aug. 4-9 (1996)
 - Workshop Fellowship
 1. Theoretical and Computational Nanoscience Workshop workshop at Oak Ridge National Laboratory, sponsored by Nanomaterial Theory Institute (2003), Oak Ridge TN (2003)
 2. ACTS workshop at Lawrence Berkeley Laboratory, sponsored by National Energy Research Supercomputer Center (NERSC), Berkeley CA (2000)

Synergetic Activities

- Software development:
I have developed several programs at the Electronic Structure Group of UMKC: (1) update the legacy Fortran 77 code of the orthogonalized linear combination of atomic orbitals (OLCAO) program to Fortran 90 standard; (2) develop a geometry optimization algorithm for OLCAO; (3) improve several key algorithms in the OLCAO program and parallize it using MPI library; (4) develop an efficient XANES/ELENS algorithm for complex system; (5) automate the calculations of XANES/ELNES, elastic properties, vibrational properties and dielectric properties using scripts; (6) develop "Xband", a color electronic and vibrational energy bands visualization programs.
- Professional activities:
I have been developing, building and maintaining electronic structure group's computational laboratory for six years. I have self built two clusters and one SAN storage network using out-of-shelf components. I am also in charge of the Sun Enterprise Server at the computer science department. I am a regular user of Department of Energy supercomputer resources. I was recently awarded 10,000 PSU of NCSA supercomputer time. I have also served as referee for Physics Review, Journal of American Ceramic Society and Journal of Applied Physics.
- Collaborations:
I collaborate with experimental scientists in my departments and other universities. Most of my collaborations focused with complex problems such bio-inspired materials and solid-solid and solid-liquid interfaces. My researches are complementary and instructive to their experimental works.

References

Curators' Prof. Wai-Yim Ching
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