

Curriculum Vitae

HUI LI

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EDUCATIONAL AND PROFESSIONAL HISTORY

2006-present Assistant professor, Department of Chemistry, University of Nebraska-Lincoln
2004-2006 Postdoctoral associate, Iowa State University, Sponsor: Prof. Mark S. Gordon
2004 Ph.D., The University of Iowa, Advisor: Prof. Jan H. Jensen
1996 M.E. in nuclear chemistry, China Institute of Atomic Energy, Beijing
1993 B.S. in chemistry, Lanzhou University, China

FELLOWSHIPS AND AWARDS

Predoctoral Fellowship, Center for Biocatalysis and Bioprocessing, The University of Iowa, 2001-2004

Leeper Award, Department of Chemistry, The University of Iowa, 2002

FULL LIST OF PUBLICATIONS

27. Hui Li "Interactions in Type-1 Cu Center", *mss in preparation*
26. Yali Wang and Hui Li "Continuous and Smooth Potential Energy Surface for Cavitation, Dispersion and Repulsion Energies in Continuum Solvation Model", *mss in preparation*
25. Peifeng Su and Hui Li "Protonation of Type-1 Cu Bound Histidines: A Theoretical Study", *mss in preparation*
24. Dejun Si and Hui Li "Quantum Chemical Calculation of Type-1 Cu Reduction Potential", *mss in preparation*
23. Dejun Si and Hui Li "Heterogeneous Conductor-Like Solvation Model", *Submitted*.
22. Peifeng Su and Hui Li "Energy Decomposition Analysis of Covalent Bonds and Intermolecular Interactions", *Submitted*.
21. Hui Li, Dmitri G. Fedorov, Takashi Nagata, Kazuo Kitaura, Jan H. Jensen and Mark S. Gordon "Solvation Energy Gradients in Combined Fragment Molecular Orbital and Polarizable Continuum Model (FMO/PCM) Calculation" *Journal of Computational Chemistry, in press*
20. Peifeng Su, Hui Li "Continuous and Smooth Potential Energy Surface for Polarizable Continuum Model Using Fixed Points with Variable Areas" *Journal of Chemical Physics*, 2009, 130, 074109
19. Jan H. Jensen and Hui Li "Calculation of Reduction Potential and pK_a " *Computational Inorganic and Bioinorganic Chemistry* (a book edited by Edward Solomon), Wiley
18. Hui Li, Jerry A. Boatz and Mark S. Gordon, "Cation-cation π - π stacking in small ionic clusters of 1,2,4-triazolium", *Journal of the American Chemical Society (Communication)*, 2008, 130, 392-393
17. Mark S. Gordon, Lyudmila V. Slipchenko, Hui Li, and Jan H. Jensen "The Effective Fragment Potential: A General Method for Predicting Intermolecular Forces", Chapter 10 in *Annual Reports in Computational Chemistry 3*, Elsevier 2007.
16. Todd J. Dolinsky, Paul Czodrowski, Hui Li, Jens E. Nielsen, Jan H. Jensen, Gerhard Klebe, Nathan A. Baker, "PDB2PQR: Expanding and upgrading automated preparation of biomolecular structures for molecular simulations", *Nucleic Acids Research*, 2007, 1-4
15. Hui Li and Mark S. Gordon, "Polarization Energy Gradients in Combined Quantum Mechanics, Effective Fragment Potential and Polarizable Continuum Model Calculations", *Journal of Chemical Physics*, 2007, 126, 124112

14. Hui Li, Heather M. Netzloff and Mark S. Gordon, "Gradients of the Polarization Energy in the Effective Fragment Potential Method", *Journal of Chemical Physics*, 2006, 125, 194103
13. Hui Li, Mark S. Gordon and Jan H. Jensen, "Charge Transfer Interaction in the Effective Fragment Potential Method", *Journal of Chemical Physics*, 2006, 124, 214108
12. Dmitri G. Fedorov, Kazuo Kitaura, Hui Li, Jan H. Jensen and Mark S. Gordon, "The Polarizable Continuum Model Interfaced with the Fragment Molecular Orbital Method", *Journal of Computational Chemistry*, 2006, 27, 976-985
11. Hui Li and Mark S. Gordon, "Gradients of the Exchange-Repulsion Energy in the Effective Fragment Potential Method", *Theoretical Chemistry Accounts*, 2006, 115, 385-390
10. Ivana Adamovic, Hui Li, Monica Lamm and Mark S. Gordon, "Modeling Styrene-Styrene Interactions", *Journal of Physical Chemistry A*, 2006, 110, 519-525
9. Hui Li, Andrew D. Robertson and Jan H. Jensen, "Very Fast Empirical Prediction and Rationalization of Protein pK_a Values", *Proteins*, 2005, 61, 704-721
8. Jan H. Jensen, Hui Li, Andrew D. Robertson and Pablo A. Molina, "Prediction and Rationalization of Protein pK_a Values Using QM and QM/MM Methods", *Journal of Physical Chemistry A* (invited feature article), 2005, 109, 6634-6643
7. Hui Li, Simon P. Webb, Joseph Ivanic and Jan H. Jensen, "The Determinants of Relative Reduction Potentials of Type-1 Copper Sites in Proteins", *Journal of the American Chemical Society*, 2004, 126, 8010-8019
6. Hui Li and Jan H. Jensen, "Improving the Efficiency and Convergence of Geometry Optimization with Polarizable Continuum Model: Energy Gradients and Molecular Surface Tessellation", *Journal of Computational Chemistry*, 2004, 25, 1449-1462
5. Hui Li, Andrew D. Robertson and Jan H. Jensen, "The Determinants of Carboxyl pK_a Values in Turkey Ovomuroid Third Domain", *Proteins*, 2004, 55, 689-704
4. Pablo A. Molina, Hui Li and Jan H. Jensen, "Intra-Protein Electrostatics From First Principles: Divide-and-Conquer Methods for QM/MM Calculations", *Journal of Computational Chemistry*, 2003, 24, 1971-1979
3. Hui Li, Christian S. Pomelli and Jan H. Jensen, "Continuum Solvation of Large Molecules Described by QM/MM: A Semi-Iterative Implementation of the PCM/EFP Interface", *Theoretical Chemistry Accounts*, 2003, 109, 71-84
2. Hui Li, Alexander Hains, Joshua Everts, Andrew D. Robertson and Jan H. Jensen, "The Prediction of Protein pK_a's Using QM/MM: The pK_a of Lysine 55 in Turkey Ovomuroid Third Domain", *Journal of Physical Chemistry B*, 2002, 106, 3486-3494
1. Hui Li and Jan H. Jensen, "Partial Hessian Vibrational Analysis: the Localization of the Molecular Vibrational Energy and Entropy", *Theoretical Chemistry Accounts*, 2002, 107, 211-219

SOFTWARE DEVELOPMENT

GAMMESS: Parts of the following methods in GAMMESS:

1. Partial Hessian Vibrational Analysis (PHVA)
2. Polarizable Continuum Model (PCM)
3. Effective Fragment Potential (EFP)
4. Localized Molecular Orbital Energy Decomposition Analysis (LMOEDA)

PROPKA: a program for fast protein pK_a prediction and analysis.

ACADEMIC MEMBERSHIP

The American Chemical Society (Division of Physical Chemistry; Division of Computers in Chemistry)