Zheng Ma

Duke University
Department of Chemistry
FFSC Room-5531, 124 Science Drive
Durham, NC, 27708

Phone: (919) 606-1611
Email: zheng.ma@duke.edu
Homepage: http://zanecode.io

Education

B.S. in Chemical Physics, University of Science and Technology of China, 2010.

Ph.D. in Computational Chemistry, Duke University, 2017 (expected).

Research Experiences

Jul.2011 - present, Computational Chemistry Group, Duke University

Research Advisor: Prof. David Beratan

1. Theoretically examined the feasibility of using two-dimensional IR spectroscopy to track electron transfer (ET) pathways;
2. Performed quantum chemistry simulation on various candidate transition-metal complex compounds in searching for vibrationally gated ET reactions;
3. Investigated the underlying mechanism of vibrationally gated ET reactions in DNA systems and established a theory framework for explaining these perturbations;
4. Established NEqMD, a methodology that enables one to use classical molecular dynamics simulation to study molecular/ensemble behavior after matter-radiation interaction in ps time scale;
5. Designed, implemented and test NEqMD-ToolKit, a Unix/Linux command-line tool kit for assisting the preparation, data collection, data mining and other related calculations in NEqMD simulations

Dec. 2010 - Jul. 2011, Magnetic Resonance Imaging Group, Duke Univ. Medical Center

Research Advisor: Prof. Warren S. Warren

1. MR imaging of Iron-based nano-particles using hyperpolarized ^{3}He and ^{129}Xe in mouse lung in searching for lung cancer cells;

Aug. 2009 - Jul. 2010 (undergraduate), Laser Chemistry Group, Hefei National Laboratory for Physical Sciences at the Microscale (HFNL)

Research Advisor: Prof. Shilin Liu

1. Studied conformational isomers of ethanol molecule and corresponding distribution in tetrachloride solution phase using Raman spectroscopy with the assistance of quantum molecular simulation.
2. Investigated solvent effect on O-H stretching motion of alcohol in polar and non-polar solvent system with help of Molecular Dynamics simulation.

Publications

Journal Articles

Z. Ma, P. Antoniou, P. Zhang, S. S. Skourtis and D. N. Beratan, "Vibrational Control of Electron Transfer: A Non-Equilibrium Molecular Dynamics Study", *in preparation*

Z. Ma, P. Antoniou, P. Zhang, S. S. Skourtis and D. N. Beratan, "Theoretical Analysis of Vibrationally Controlled Electron Transfer Reactions", *in preparation*

P. Antoniou, Z. Ma, P. Zhang, D. N. Beratan, S. S. Skourtis, "Vibrational Control of Electron-Transfer Reactions: A Feasibility Study For The Fast Coherent Transfer Regime", *Phys. Chem. Chem. Phys*, **2015**, 17, 30854-30866

Y. Yue, T. Grusenmeyer, Z. Ma, P. Zhang, RH Schemhl, D. N. Beratan, I. V. Rubtsov; "Electron Transfer Rate Modulation in a Compact Re(I) Donor-Acceptor Complex" *Dalton Transactions*, **2015**, 44, 8609-8616

Y. Yue, T. Grusenmeyer, Z. Ma, P. Zhang, RH Schemhl, D. N. Beratan, I. V. Rubtsov; "Full-Electron Ligand-to-Ligand Charge Transfer in a Compact Re(I) Complex", *J. Phys. Chem. A*, **2014**, 118, 10407-10415

Y. Yue, T. Grusenmeyer, Z. Ma, P. Zhang, T. T, Pham, J. T. Mague, J. P. Donahue, R. H. Schmehl, D. N. Beratan, I. Rubtsov; "Evaluating the Extent of Intramolecular Charge Transfer in the Excited States of Rhenium(I) Donor-cceptor Complexes with Time-Resolved Vibrational Spectroscopy", *J. Phys. Chem. B*, **2013**, 117, 15903-15916

M. Freeman, K. Claytor, Y. Qi, S. Degan, Z. Ma, W. S. Warren, B. Driehuys, R. T. Branca; "Hyperpolarized ^{129}Xe And ^{3}He MRI For Sensitive Detection Of Iron Oxide Contrast In The Mouse Lung", *Am J Respir Crit Care Med*, **2012**, 185:A2250