

# Weijie HUA

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ResearchID: F-3099-2010

- PERSONAL     ◇ Male, born in 1982 in Jiangsu, P. R. China. Chinese citizen.  
                 ◇ Married, with one child.
- EDUCATION   ◇ 2007.12-2011.04, Ph.D. degree in Biotechnology under the direction of Prof. Yi Luo, Royal Institute of Technology, Sweden.  
                 Thesis title: *Structure and spectroscopy of bio- and nano-materials from first-principles simulations*.  
                 ◇ 2004.09-2010.11, Ph.D. degree in Physical Chemistry under the direction of Prof. Shuhua Li, Nanjing University, China.  
                 Thesis title: *Approximate methods for calculating ground-state electronic structure and properties of large molecules: methodological developments and applications*.  
                 ◇ 2000.09-2004.07, B.S. degree in Chemistry, Nanjing University, China.
- EMPLOYMENT ◇ 2011.05-present, postdoctoral fellow with Prof. Yi Luo in Royal Institute of Technology, Sweden.
- AWARDS       ◇ 2007-2009, Scholarship "High-level Government-Sponsored Overseas Study Program" from China Scholarship Council.  
                 ◇ 2001, Provincial (1st place) award from the National Mathematical Modelling Contest.  
                 ◇ 2000-2004, Peoples' Scholarship, Nanjing University.
- RESEARCH INTERESTS     ◇ X-Ray Science, Electronic Structure Theory, Spectroscopy and Properties, Simulation.
- RESEARCH EXPERIENCE   ◇ **X-ray chemistry**, especially soft x-ray spectroscopy calculations for bio-/nano- materials.  
                 ◇ **Molecular fragmentation method for large molecules**, especially development and application of the generalized energy-based fragmentation (GEBF) method for property/spectroscopy calculations.  
                 ◇ **Simulations**, classical or ab initio Monte Carlo/molecular dynamics simulations for complex systems, simple solutions, and polymers.  
                 ◇ **Magnetochemistry**, especially model Hamiltonian and quantum mechanical calculations for single molecular magnets.
- SOFTWARE CONTRIBUTION   ◇ Shuhua Li\*, Wei Li, Tao Fang, Jing Ma, Weijie Hua, Shugui Hua, and Yuansheng Jiang, Lower Scaling Quantum Chemistry (LSQC) Program, version 2.0, Nanjing University, Nanjing, 2010, <http://itcc.nju.edu.cn/lsgc>.  
                 ◇ Guangjun Tian, Sai Duan, Weijie Hua, Yi Luo\*, DynaVib, version 1.0, Royal Institute of Technology, Stockholm, 2012.
- TECHNICAL EXPERTISE     ◇ Familiar programming languages/script:  
                 MATLAB (11 years), FORTRAN (8 years), C, BASH.  
                 ◇ Softwares:  
                 Electronic structure and properties: GAUSSIAN, GAMESS-US, ORCA, DALTON, TURBOMOLE, ADF; X-ray spectra: STOBE, BIO-NANO LEGO; Molecular dynamics: CPMD, VASP, DYNAMO, MDYNAMIX, AMBER; semi-empirical: MOPAC.

PUBLICATION  
LIST◇ **X-ray spectroscopy**

These papers have investigated soft x-ray spectroscopies, with emphasis of the NEXAFS, of biomolecules and nano-materials. Good agreement with the experimental spectra and further explanations have been highlighted.

1. X-ray Absorption Spectra of graphenes from first-principles simulations.  
W. Hua, B. Gao, S. Li, H. Ågren, and Y. Luo, *Phys. Rev. B* **2010**, 82, 155443.
  2. Systematic study of soft-X-ray spectra of poly(dG)·poly(dC) and poly(dA)·poly(dT) DNA duplexes.  
W. Hua, H. Yamane, B. Gao, J. Jiang, S. Li, H. S. Kato, M. Kawai, T. Hatsui, Y. Luo, N. Kosugi, and H. Ågren, *J. Phys. Chem. B* **2010**, 114, 7016.
  3. Refinement of DNA structures through NEXAFS analysis: applications on guanine and cytosine nucleobases, nucleosides and nucleotides.  
W. Hua, B. Gao, S. Li, H. Ågren, and Y. Luo, *J. Phys. Chem. B* **2010**, 114, 13214.
  4. X-ray spectroscopy of blocked alanine in water solution from supermolecular and supermolecular-continuum solvation models: A first-principles study.  
W. Hua, Y.-J. Ai, B. Gao, H. Li, H. Ågren, and Y. Luo, *Phys. Chem. Chem. Phys.* **2012**, 000, 0000.
  5. First-Principles Simulation of Soft X-Ray Spectroscopy.  
W. Hua, B. Gao, and Y. Luo, *Progress in Chemistry* **2012**, 000, 0000. (review).
  6. Theoretical study of two  $I_h$ -symmetry-breaking  $C_{60}$  isomers and their chlorinated species in core-excited and ground states  
J. Qi, W. Hua, B. Gao, *Chem. Phys. Lett.* **2012**, 000, 0000.
  7. First Principles Study on Core-Level Spectroscopy of Arginine in Gas and Solid Phases  
H. Li, W. Hua, Z. Lin, and Y. Luo, *J. Phys. Chem. B*, in review.
  8. Theoretical study of core excitations of fullerene-based solar cell acceptors  
X. Song, W. Hua, Y. Ma, C. Wang, and Y. Luo, *Phys. Chem. Chem. Phys.*, submitted.
- ◇ **Molecular fragmentation method for large molecules**
- These papers challenge the first-principles property (energy, structure, infrared and Raman spectra) calculations for large molecules by using the generalized energy-based fragmentation (GEBF) method. Both methodological developments and applications in biomolecules, nanotubes, and water clusters have been made.
9. Geometry optimizations and vibrational spectra of large molecules from a generalized energy-based fragmentation approach.  
W. Hua, T. Fang, W. Li, J.-G. Yu, S. Li, *J. Phys. Chem. A* **2008**, 112, 10864.
  - \*. Understanding the accuracy of the generalized energy-based fragmentation approach at the Hartree-Fock level by multipole expansion analysis.  
W. Hua, W. Li, Y. Guo, Shuhua Li, Yi Luo, *in manuscript*
  10. The energy-based fragmentation approach for computing total energies, structures, and molecular properties of large systems at the ab initio levels, in Jeffrey R. Reimers (ed.), *Computational Methods for Large Systems: Electronic Structure Approaches for Biotechnology and Nanotechnology*.  
W Li, W. Hua, F. Tao, S. Li, John Wiley & Sons Inc., **2011**, pp. 182-210.

11. An efficient implementation of the generalized energy-based fragmentation approach for general large molecules.  
S. Hua, W. Hua, and S. Li, *J. Phys. Chem. A* **2010**, 114, 8126.
  12. Low-lying structures and stabilities of large water clusters: investigation based on the combination of the AMOEBA potential and generalized energy-based fragmentation approach.  
Z. Yang, S. Hua, W. Hua, and S. Li, *J. Phys. Chem. A* **2010**, 114, 9253.
  13. Structures of Neutral and Protonated Water Clusters Confined in predesigned hosts: A Quantum Mechanical/Molecular Mechanical study, Z. Yang, S. Hua, W. Hua, and S. Li, *J. Phys. Chem. B* **2011**, 115, 8249.
- ◇ **Model Hamiltonian and magnetochemistry**  
These papers are extensive cooperations with inorganic experimentalists. The theoretical part includes fitting of the magnetic susceptibility-temperature relation to the Van Vleck equation by using the Heisenberg model and broken-symmetry quantum chemistry calculations.
14. Experimental and theoretical magneto-structural studies on the dicarboxylato-bridged nature of the dicopper(II)-based metal-organic frameworks,  
M.-S. Chen, W.-J. Hua, Y. Song, P. Wang, W.-Y. Sun, C.-Y. Zhang, G.-X. Zeng, S.-H. Li, *Inorg. Chim. Acta.*, **2012**, 387, 137–144.
  15. A supramolecular assembly of {Fe}<sub>10</sub> molecular wheels with tubular structures,  
G. Q. Jiang, Y. Z. Li, W. Hua, Y. Song, J. F. Bai, S. Li, M. Scheer, X. You, *CrystEngComm* **2006**, 8, 384.
  16. Metal complexes formed by metal-assisted solvolysis of di-2-pyridylketone azone: structures and magnetic properties  
D. Wu, W. Huang, W. Hua, Y. Song, C. Duan, S. Li, and Q. Meng, *Dalton. Trans.* **2007**, 18, 1838.
  17. Tetranuclear manganese(III) clusters containing both carboxylate and phosphonate bridging ligands  
Y.-S. Ma, H.-C. Yao, W. Hua, S. Li, Y.-Z. Li, L.-M. Zheng, *Inorg. Chim. Acta.* **2007**, 360, 1645.
- \*. Diruthenium(III,III) Diphosphonate with Large Negative Zero Field Splitting: An Experimental and DFT Study,  
B. Liu, J. Jin, W.-J. Hua, H.-M. Hu, L.-M. Zheng, S.-H. Li, in manuscript.
- ◇ **Simulations**  
These papers are application works on host-guest systems, confined systems, and polymers. Monte Carlo, molecular dynamics simulations or cluster-model calculations employing pure QM, hybrid QM/QM', and model Hamiltonians are covered.
18. Understanding the influence of the guest-host interaction on the conformations of short peptides in the hydrophobic cavity: A computational study,  
W. Hua, L. Xu, Y. Luo, S. Li, *ChemPhysChem* **2011**, 12, 1325.
  19. Estimating on the individual hydrogen bond in molecules with multiple hydrogen bonds  
H. Dong, W. Hua and S. Li, *J. Phys. Chem. A* **2007**, 111, 2941.  
(One of the ACS's Most-Accessed Articles, April-June, 2007)
  20. A large protonated water cluster H<sup>+</sup>(H<sub>2</sub>O)<sub>27</sub> in a 3D metal-organic framework,  
M. Wei, C. He, W. Hua, C. Duan, S. Li, and Q. Meng, *J. Am. Chem. Soc.* **2006**, 128, 13319.

- \*. Monte carlo simulations of polymer configurations in dilute solution, W. Hua, undergraduate dissertation, Nanjing University, Nanjing **2004**.

◇ **Other**

21. Spectroscopic constants of single-bond diatomic molecules and singlet-triplet gaps of di-radicals by the block-correlated coupled cluster theory.  
J. Shen, T. Fang, W. Hua, S. Li, *J. Phys. Chem. A* **2008**, 102, 4703.
22. Repair of DNA Dewar photoproduct to (6-4) photoproduct in (6-4) photolyase, Y.-J. Ai, R.-Z. Liao, S.-L. Chen, W. Hua, W.-H. Fang, Y. Luo, *J. Phys. Chem. B* **2011**, 115, 10976.

REFEREES

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- ◇ Shuhua Li, professor  
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(Updated: May 8, 2012)