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Personal Information Zheng Wenrui, female,Ph.D, awarded from University of Science and Technology of China. Associate Professor, School of Chemistry and Chemical Engineering, Shanghai University of Engineering Science. +86-21-67791216, wrzheng@sues.edu.cn. Research Fields The research interests are quantum chemical calculations and physical organic chemistry with the directions including: 1. the thermodynamics basis on the inert chemical bond activation; 2. the hydrogen bonding interaction in organic catalysis; 3. the precision calculations on bond dissociation enthalpy of organic compounds. Research Achievements 1. Zheng, W. R.; Xu, W. X.; Wang, Y. X.; Chen, Z. C. Computational and Theoretical Chemistry, 2014, 1027, 116. 2. Zheng, W. R.; Chen, Z. C.; Xu, W. X. Chinese Journal of Chemical Physics, 2013, 26, 541. 3. Zheng, W. R.; Chen, Z.-C.; Xu, J. L.; Yang, Q.; Huang, T. Journal of Sulfur Chemistry 2012, 33, 541. 4. Zheng, W. R.; Guo, Z. L.; Chen, Z. C.; Yang, Q.; Huang, T. Res Chem Intermed 2012, 38, 1791. 5. Zheng, W. R.; Xu, J. L.; Huang, T.; Chen, Z.-C.; Yang, Q. Computational and Theoretical Chemistry 2011, 968, 1. We are hiring Postdoc and PhD students who are interested in the following directions: 1. Epitaxial thin film growth/design for transparent conductive oxides 2. Wide bandgap semiconductor and electronic devices 3. Carrier transport in solar energy conversion Please send your CV directly to zhangwenrui@nimte.ac.cn We synthesize functional materials and enable their applications for advanced solid-state devices and renewable energy conversion. We strive to perfect the growth of thin films and heterostructures, and control the fundamental building blocks with atomic-level precision. The improved capability of precise materials synthesis allows us to explore emerging phenomena in correlated electron systems from bulk to interface, and to drive the development of novel information technology. In parallel, we explore exotic carrier transport and dynamics in model semiconductors, with an aim to accelerate materials design and discovery for efficient solar energy conversion. Ph.D. Materials Science and Engineering Texas A&M University (TAMU) 2011-2015 B.S. Materials Science and Engineering Wuhan University of Science & Technology (WUST) 2007-2011 -Outstanding Oral Presentation Award (Consecutively), Early Career Research Symposium, BNL, 2018, 2017 -Outstanding Reviewer Award, Institute of Physics Publishing (Journal of Physics D: Applied Physics), 2017 -Best Poster Award, NSLS-II and CFN Users' Meeting, BNL, 2017 -Graduate Travel Grant, TAMU, 2013 -First-grade Outstanding Student Scholarships, Top 3%, WUST, 2007-2011 -Xu Jiayin Scholarship, WUST, 2010 Staff Scientist: Ningbo Institute of Materials Technology & Engineering (NIMTE), Chinese Academy of Sciences 2020-Current Postdoc Research Associate: Oak Ridge National Laboratory (ORNL) Project: Correlated Electron Systems and Low Dimensional Materials Advisor: Dr. Gyula Eres and Dr. Thomas Zac Ward 2018-2020 Postdoc Research Associate: Brookhaven National Laboratory (BNL) 2016-2018 Project: Exotic Transport in Semiconductors for Solar Fuel Production Advisor: Dr. Mingzhao Liu 2016-2018 Graduate Research Assistant: Texas A&M University Project: Ferroic Functionalities Achieved by a Vertically Aligned Nanocomposite Approach Advisor: Prof. Haiyan Wang 2011-2015 Advisory Panel for Journal of Physics D: Applied Physics 2018-Current Proposal Review Panel for DOE NSRC program 2019-Current Reviewer for 30+Journals: - Science Advances, Nature Communications, Advanced Materials - ACS Applied Materials & Interfaces, - Journal of Materials Chemistry A, Journal of Materials Chemistry C, Chemical Communications - Materials Research Letters, Applied Physics Letters, APL Materials, Journal of Applied Physics, Journal of Physics D: Applied Physics, Journal of Physics: Condensed Matters, - Nanotechnology, Materials & Design, Applied Surface Science, Materials Science and Engineering A, - Scientific Reports, Polymers, Journal of Magnetism and Magnetic Materials, Nanoscale Research Letters, Thin Solid Films, Vacuum, Materials Research Express, Surface Review and Letters. 代表性论著 (论文、著作、专利) 1. Huifang Chang, Wenrui Zheng*, Yuanyuan Zheng, Danfeng Zhu, Jiaoyang Wang. The DFT study on Rh–C bond dissociation enthalpies of (iminoacyl) rhodium(III)hydride and (iminoacyl)rhodium(III)alkyl. Tetrahedron Letters2019, 60, 310-321.2. Yuanyuan Zheng, Wenrui Zheng*,Jiaoyang Wang, Huifang Chang, Danfeng Zhu. Computational study on N−N homolytic bond dissociation enthalpies of hydrazine derivatives. J. Phys. Chem. A2018, 122, 2764−2780.3. Jiaoyang Wang, Wenrui Zheng*, Yuanyuan Zheng. Theoretical study on homolytic B–B cleavages of diboron(4) compounds. RSC Adv. 2017, 7, 49251-49272.4. Jiaoyang Wang, Wenrui Zheng*, Lanlan Ding, Yingxing Wang. Computational study on C–B homolytic bond dissociation enthalpies of organoboron compounds. New J. Chem., 2017, 41, 1346-1362.5. Wenrui Zheng*, Lanlan Ding, Jiaoyang Wang, Yingxing Wang. Computational study on alkenyl/aryl C(sp2)–O homolytic cleavage of carboxylates and carbamates. RSC Adv.2016, 6, 26514-26525.6. Yingxing Wang, Wenrui Zheng*, Lanlan Ding. The C–H Bond dissociation enthalpies in fused N-heterocyclic compounds. Russian Journal of Physical Chemistry A2016, 90(3), 610-621.7. Lanlan Ding, Wenrui Zheng*, Yingxing Wang. Theoretical study on homolytic C(sp2)–O cleavage in ethers and phenols. NewJ. Chem., 2015, 39, 6935-6943.8. Lanlan Ding, Wenrui Zheng*, Yingxing Wang. The homolytic C-O cleavage in phosphates and sulfonates. J. Phys. Chem. A, 2015,119, 3488-3499.9. Yingxing Wang, Wenrui Zheng*. A comparison of the C–H bond dissociation enthalpies of sulfur-containing fused heterocyclic compounds to the C–H bond dissociation enthalpies in other heterocycles. Journal of Sulfur Chemistry, 2015, 36, 155-169.10. Yingxing Wang, Wenrui Zheng*. A theoretical study on C–H bond dissociation enthalpies of oxygen-containing fused heterocyclic compounds. Res Chem Intermed, 2015, 41, 7207-7225.11. Wenrui Zheng*, Wuxia Xu, Yingxing Wang, Zhichong Chen. 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Res Chem Intermed2011, 37, 31-45.17. Wenrui Zheng*, Jingli Xu, Rui Xiong. Density functional theory study on N-O bond dissociation enthalpies. Acta Phys. -Chim. Sin.2010, 26(9), 2535-2542.18. Wenrui Zheng, Yao Fu, Lei Liu, Qingxiang Guo*. G3//BMK and its application to calculation of bond dissociation enthalpies. J. Chem. Theory Comput.2008, 4, 1324-1331.19. Wenrui Zheng, Yao Fu, Huajing Wang, Qingxiang Guo*. C-H bond dissociation enthalpies of hydrocarbons by DFT studies. Chin. J. Org. Chem.2008, 28(3), 459-466.20. Wenrui Zheng, Yao Fu, Kuang Shen, Lei Liu, Qingxiang Guo*. Theoretical study on hydrogen bonding interaction of ureas and thioureas with imines. Journal of Molecular Structure: THEOCHEM2007, 822, 103-110.21. Wenrui Zheng, Yao Fu, Lei Liu, Qingxiang Guo*. Hydrogen bonding interaction between ureas or thioureas and carbonyl compounds. Acta Phys. -Chim. Sin.2007, 23(7), 1018-1024. This question is for testing whether you are a human visitor and to prevent automated spam submission. Audio is not supported in your browser. What code is in the image? Your support ID is: 8203162017352035351. Research Fellows Dr Zheng, Wenrui B. Sc. Huazhong University of Science and Technology Ph. D. National University of Singapore Email: e0220130@u.nus.edu Dr He, Rongde B. Sc. Shenyang University of Chemical Technology Ph. D. Lanzhou University Email: herd@nus.edu.sg Dr Shen, Zi-An (NUS Suzhou Research Institute) B. Sc. Sichuan University Ph. D. National University of Singapore Email: e0444171@u.nus.edu Dr Zhu, Kun (NUS Suzhou Research Institute) B. Sc. Nankai University Ph. D. National University of Singapore Email: e0444227@u.nus.edu Dr Wu, Zugen B. Sc. Fudan University Ph. D. National University of Singapore Email: zugen.wu@u.nus.edu Ph.D. Students Sun, Yuli NUS-TJU Research Scholar B. Sc., M. Sc. 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ShanghaiTech University Email: e1353460@u.nus.edu Wang, Kuiyang Dean's Graduate Fellowship B. Sc. Shanghai Jiao Tong University Email: e1353384@u.nus.edu Master Students Gao, Ping B.Sc. Southwest university Email:e1350002@u.nus.edu Gu , Zhongjin B.Eng. Jiangsu Normal University Email:e1350163@u.nus.edu Zhou , Yuxuan B.Eng. Tongji University Email: e1350207@u.nus.edu Wang, Yifan B.Sc. The University of Hong Kong Email: e1349543@u.nus.edu Li, Chenyu B. Eng. Sichuan University Email: e1352234@u.nus.edu Zhang , Huiwen B.Sc. Dalian University of Technology Email: e1348878@u.nus.edu Liu , Leyan B.Sc. Dalian University of Technology Email: e1353383@u.nus.edu