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中山大學中法核工程与技术学院

Institut franco-chinois de l'énergie nucléaire université Sun Yat-sen

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教育经历

- 2008.09 – 2013.07 清华大学，化学，理学博士
2011.12 – 2012.11 赫尔辛基大学，理论与计算化学
2005.09 – 2008.07 中国矿业大学，物理化学，理学硕士
2001.09 – 2005.07 中国矿业大学，应用化学，理学学士

工作经历

2018.04 – 2018.12 名古屋大学, ITbM研究员
2017.10 – 2018.03 分子科学研究所(日本), 分子科学研究所(IMS)研究员
2016.04 – 2017.03 分子科学研究所(日本), 日本学术振兴会(JSPS)研究员
2013.08 – 2017.09 中国科学院上海应用物理研究所, 助理研究员

研究方向

理论与计算化学, 铜系化学

国家自然科学基金青年项目

含氮杂环钆(III)配合物电子结构与化学成键的理论研究 (No. 21501189), 项目负责人

文章著作

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9. Takeshi Yanai^{*}, Masaaki Saitow, **Xiao-Gen Xiong**, Jakub Chalupský, Yuki Kurashige, Sheng Guo, and Sandeep Sharma. Multistate complete-active-space second-order perturbation theory based on density matrix renormalization group reference states. *Journal of Chemical Theory and Computation*, 2017, 13, 4829–4840.
10. **Xiao-Gen Xiong**^{*} and Takeshi Yanai^{*}. Projector Augmented Wave Method Incorporated into Gauss-type Atomic Orbital Based Density Functional Theory. *Journal of Chemical Theory and Computation*, 2017, 13, 3236–3249.
11. Cong-Qiao Xu, **Xiao-Gen Xiong**, Wan-Lu Li, and Jun Li^{*}. Periodicity and Covalency of [MX₂]⁻ (M = Cu, Ag, Au, Rg; X = H, Cl, CN) Complexes. *European Journal of Inorganic Chemistry*, 2016, 1395 – 1404.
12. Xiaojing Guo^{*}, **Xiao-Gen Xiong**, Cheng Li, Hengfeng Gong, Ping Huai, Jiangtao Hu, Chan Jin, Liangliang Huang and Guozhong Wu^{*}. DFT investigations of uranium complexation with amidoxime-, carboxyl- and mixed amidoxime/carboxyl-based host architectures for sequestering uranium from seawater. *Inorganica Chimica Acta*, 2016, 441, 117 - 125.
13. Han Han^{*}, Cheng Cheng, **Xiao-Gen Xiong**, Jing Su, Jian-Xing Dai, Hui Wang, Gen Yin and Ping Huai^{*}. Piezoelectric, Mechanical and Acoustic Properties of KNaNbOF₅ from First-Principles Calculations. *Materials*, 2015, 8(12), 8578 - 8589.
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15. **Xiao-Gen Xiong**, Wenhua Xu, Jun Li^{*} and Pekka Pyykkö^{*}. Aspects of bonding in small gold clusters. *International Journal of Mass Spectrometry*, 2013, 354-355, 15-18.
16. Hong-Tao Liu, **Xiao-Gen Xiong**, Phuong Diem Dau, Yi-Lei Wang, Dao-Ling Huang, Jun Li^{*} and Lai-Sheng Wang^{*}. Probing the Nature of Au-C bonding in Alkynyl-Gold(I) Complexes. *Nature Communications*, 2013, doi:10.1038/ncomms3223.
17. **Xiao-Gen Xiong** and Pekka Pyykkö^{*}. Unbridged Au(II)-Au(II) bonds are theoretically allowed. *Chemical Communications*, 2013, 49, 2103-2105.
18. Chuan-Gang Ning, **Xiao-Gen Xiong**, Yi-Lei Wang, Jun Li^{*} and Lai-Sheng Wang^{*}. Probing the electronic structure and chemical bonding of the "staple" motifs of thiolate gold nanoparticles: Au(SCH₃)⁻₂ and Au₂(SCH₃)⁻₃. *Physical Chemistry Chemical Physics*, 2012, 14, 9323-9329.

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