


西华大学硕士研究生导师简介

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出生年月	1985年5月	
职称/最高学历	副教授/博士	
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电话	13683449222	
招收专业	功能材料化学	
主要研究方向 (至少填一项)	理论与计算化学	
个人简介: (学历简历、工作经历、社会任职、荣誉称号、从事科研情况简介; 将科研方向内容介绍清楚)	<p>2004年6月获四川大学化学本科学位;</p> <p>2013年6月获四川大学物理化学专业博士学位;</p> <p>2013年7月到西华大学理学院参加工作, 2015年10月晋升副教授;</p> <p>2015年8月至2016年7月: 韩国仁荷大学(Inha University)自然科学院化学与化学工程系博士后。</p> <p>目前主要从事有机、催化反应机理以及相关体系催化剂分子设计等方面的科研工作。近几年作为项目负责人主持国家自然科学基金、四川省教育厅青年基金和西华大学重点项目各1项。在 Chem. Eur. J., J. Org. Chem., Org. Chem. Front., RSC Adv., 等杂志发表 SCI 收录论文 17 余篇; 其中第一作者及通讯作者的论文 11 篇。</p>	
近年作为项目负责人主持的科研项目: <ol style="list-style-type: none"> 1 水介质中 Zn 配合物催化 C=O 和 C=N 双键烯丙基化反应机理及选择性理论研究, 国家自然科学基金(青年基金), 2014.10-2017.12, 25.0 万元; 2 以 CO₂ 和氨基苄腈为原料水溶液中合成喹唑啉酮的反应机理及催化剂设计研究, 四川省教育厅 2014.03-2015.12 1.0 万元; 3 由 CO₂ 和 2-氨基苄腈合成喹唑啉-2,4(1H,3H)-二酮的反应机理研究, 西华大学校重点项目, 2013.10-2016.12, 6.0 万元; 4 计算催化循环频率(TOF)软件的开发及应用, 中国工程物理研究院物资部委托, 2015.06-2018.04, 2.5 万元。 		

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近年发表的科研论文:

1. **Weiyi Li***, Na Yang, Yajing Lyu, A mechanistic study on guanidine-catalyzed chemical fixation of CO₂ with 2-aminobenzonitrile to quinazoline-2,4(1*H*,3*H*)-dione, *Org. Chem. Front.* **2016**, 3, 823.
2. **Weiyi Li***, Na Yang, Yajing Lyu, Theoretical insights into the catalytic mechanism of N-heterocyclic olefins in carboxylative cyclization of propargyl alcohol with CO₂, *J. Org. Chem.* **2016**, 3, 5303.
3. Jun Wen, Liang Dong, Sheng Hu, **Weiyi Li***, Shuo Li*, Xiaolin Wang, Fluorogenic thorium sensors based on 2,6-Pyridinedicarboxylic acid-substituted tetraphenylethenes with aggregation-induced emission characteristics, *Chem. Asian J.*, **2016**, 11, 49.
4. Jun Wen, Zeng Huang, Sheng Hua, Shuo Li, **Weiyi Li***, Xiaolin Wang, Aggregation-induced emission active tetraphenylethene-based sensor for uranyl ion detection, *J. Hazard. Mater.* **2016**, 318, 363.
5. **Weiyi Li***, Na Yang, Yajing Lv, Theoretical study of the BINOL-zinc complex catalyzed asymmetric inverse-electron-demand imino Diels-Alder reaction: mechanism and stereochemistry, *RSC Adv.* **2015**, 5, 93318.
6. Liang Dong, Jun Wen*, **Weiyi Li***, A Theoretical investigation of substituent effects on the stability and reactivity of N-heterocyclic olefin carboxylates, *Org. Biomol. Chem.* **2015**, 11, 7497.
7. Liang Dong, Yun, Xie, Liang Du, **Weiyi Li***, Zhaoyi Tan*, Theoretical investigation of isotope exchange reaction in tritium-contaminated mineral oil in vacuum pump, *J. Hazard. Mater.* **2015**, 278, 42.
8. Liang Dong, Jiamao Li, Bing Deng, Yong Yang, Heyi Wana, **Weiyi Li**, Shuo Li, Zhaoyi Tan*, Theoretical investigation of the mechanism of tritiated methanodehydrogenation reaction using nickel-based catalysts, *Fusion Eng. Des.* **2015**, 95, 91.
9. **Weiyi Li***, Dongfeng Huang, Yajing Lv, Theoretical investigations on the mechanism of dual 1,3-Dipolar cycloaddition of CO₂ with isocyanides and alkynes, *J. Org. Chem.* **2014**, 79, 10811.
10. **Weiyi Li***, Dongfeng Huang, Yajing Lv, Mechanism of N-heterocyclic carbene-catalyzed chemical fixation of CO₂ with aziridines: a theoretical study, *RSC Adv.*, **2014**, 4, 17236.
11. **Weiyi Li***, Dongfeng Huang, Yajing Lv, Theoretical study on the mechanism and stereochemistry of the cinchona-thiourea organocatalytic hydrophosphonylation of an α -ketoester, *Org. Biomol. Chem.* **2013**, 11, 7497.
12. **Weiyi Li**, Zhishan Su and Changwei Hu*, Mechanism of allylation of ketone with allylboronates as catalyzed by zinc compounds: a DFT study, *Chem. Eur. J.* **2013**, 19, 124.
13. Zhishan Su, **Weiyi Li**, Jun Wang, Changwei Hu*, Xiaoming Feng*, Theoretical investigation on strecker reaction catalyzed by a Ti(IV)-complex catalyst generated from cinchona alkaloid, achiral substituted 2,2'-biphenol and tetrakispropyl titanate, *Chem. Eur. J.* **2013**, 19, 1637.
14. **Weiyi Li**, Song Qin, Zhishan Su, Changwei Hu*, Xiaoming Feng*, Theoretical study on the

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- mechanism and stereochemistry of salicylaldehyde–Al(III)-catalyzed hydrophosphonylation of benzaldehyde, *Comput. Theor. Chem.* **2012**, 989, 44.
15. Wei Zhang, **Weiyi Li**, Song Qin*, Origins of Enantioselectivity in the chiral diphosphine-ligated CuH-catalyzed asymmetric hydrosilylation of ketones, *Org. Biomol. Chem.* **2012**, 10, 597.
16. Bo Liu, Xiangguang Meng,* **Weiyi Li**, Liangchun Zhou, and Changwei Hu, Theoretical and experimental studies on selective oxidation of aromatic ketone by performic Acid, *J. Phys. Chem. A* **2012**, 116, 2920.
17. **Weiyi Li**, Song Qin, Zhishan Su, Huaqing Yang, Changwei Hu*, Theoretical study on the mechanism of Al(salalen)-catalyzed hydrophosphonylation of aldehydes, *Organometallics* **2011**, 30, 2095.