基本信息

姓　　名	**谢 静**
职　　务	
职　　称	准聘教授，博士生导师
研究方向	理论与计算化学
学术网站	https://www.x-mol.com/groups/jingxie
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教育背景

2010.07-2015.05	美国德克萨斯理工大学，化学专业，博士
2006.09-2010.07	北京师范大学，化学专业，学士

工作履历

2019.03-至今	北京理工大学，化学与化工学院，准聘教授
2015.06-2019.02	美国明尼苏达大学，化学系，博士后

研究方向

1.	直接动力学模拟气相反应动态机理，微溶剂化作用
2.	锂/钠离子、锂硫电池电极材料及电解质的计算模拟

荣誉奖励

1.	2018 入选北京理工大学“特立青年学者”
2.	2014 德克萨斯理工大学 Horn Professor's 研究成果奖
3.	2010 北京师范大学优秀毕业生论文，北京市优秀毕业生

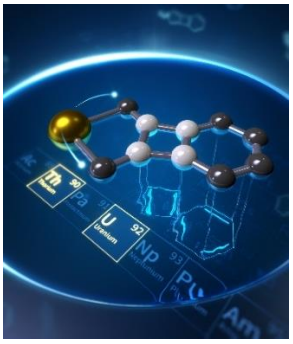
承担项目

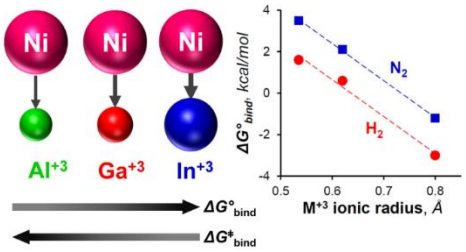
1.	北京理工大学“高层次人才科研启动计划”项目 100 万　2019.3 – 2025.2
2.	国家自然科学基金青年项目 26 万　2020.1 – 2022.12

研究成果

主持国家自然科学基金青年项目 1 项，北京理工大学“高层次人才科研启动计划”项目 1 项。迄今在 *Science, Nature, Acc. Chem. Res., J. Am. Chem. Soc., Angew. Chem. Int. Ed, Chem. Sci., Nature Chem., J. Phys. Chem., J. Chem. Phys.* 等学术期刊上发表论文 29 篇。

发表论文（代表作用红色标注）

29.	F. Ma, **J. Xie**, X. Zheng,* Z. Li.* Binding Properties of Cucurbit[7]uril to Neutral and Protonated Amino Acids: A Theoretical Study. *Int. J. Quantum Chem.* **2020** Accepted
28.	Z.Xing,# G. Tan,# Y. Yuan, B. Wang, L. Ma, **J. Xie**, Z. Li, T. Wu, Y. Ren, R. Shahbazian-Yassar, J. Lu*, X. Ji*, Z. Chen.* “Consolidating Lithiothermic-Ready Transition Metals for Li2S-Based Cathodes” *Adv. Mater.*, **2020**, 32(31), 2002403.
27.	D. Ray,# **J. Xie**,# J. White, G. E. Sigmon, L. Gagliardi, A. E. Hixon.* Experimental and quantum mechanical characterization of an oxygen-bridged plutonium(IV) dimer. *Chem. Eur. J.* **2020**, 26，8115-8120
26.	J. K. Pagano,# **J. Xie**,# K. A. Erickson, S. K. Cope, B. L. Scott, R. Wu, R. Waterman, D. E. Morris,* P. Yang,* L. Gagliardi,* J. L. Kiplinger.* Actinide 2-metallabiphenylenes that satisfy Hückel’s Rule. ***Nature* 2020**, *578*, 563-567 (#共同一作，影响因子 41.5) 相关报道 ChemistryWorld: Uranium and thorium make their debut in dual aromatic–antiaromatic molecule ChemistryViews: First Metallabiphenylene Analogues Synthesized University of Minnesota news：Scientists synthesize and characterize, for the first time, actinide 2-metalla-biphenylene compounds x-mol：Nature：符合“休克尔定律”的锕系 2-金属取代亚联苯化合物 
25.	R. C. Cammarota,# **J. Xie**,# S. A. Burgess, M. V. Vollmer, K. D. Vogiatzis, J. Ye, J. C. Linehan, A. M. Appel, C. Hoffmann, X. Wang, V. G. Young Jr, C. C. Lu.* Thermodynamic and Kinetic Studies of H_2 and N_2 Binding to Bimetallic Nickel-Group 13 Complexes and Neutron Structure of a Ni(η^2-H_2) Adduct. *Chem. Sci.* **2019**, *10*, 7029-7042 (#共同一作,影响因子 9.06)



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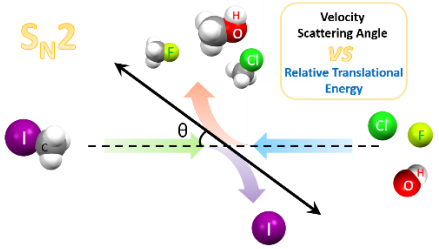

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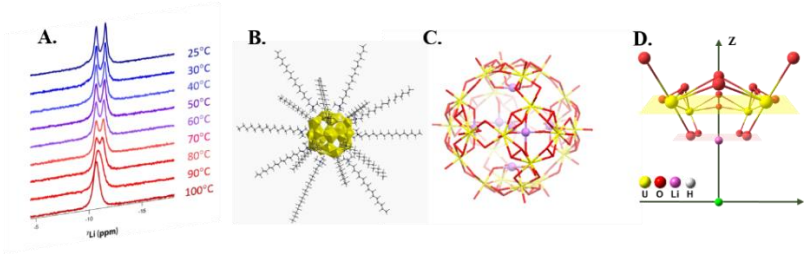
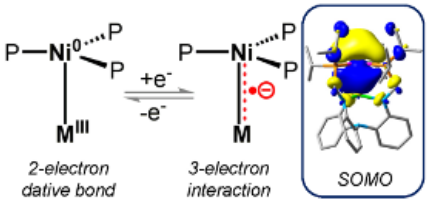


22. M. V. Vollmer,# J. Xie,# R. C. Cammarota, V. G. Young Jr., E. Bill,* L. Gagliardi,* C. C. Lu*. Formal nickelate(−I) complexes supported by group 13 ions.Angew. Chem. Int. Ed. 2018, 57, 7815-7819 (# 共同一作)



21. J. Ye,* R. C. Cammarota, **J. Xie**, M. V. Vollmer, D. G. Truhlar, C. J. Cramer, C. C. Lu,* L. Gagliardi.* Rationalizing the Reactivity of Bimetallic Molecular Catalysts for CO_2 Hydrogenation. *ACS Catal*. **2018**. 8, 4955–4968

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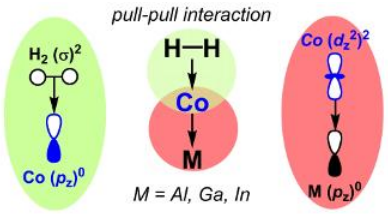
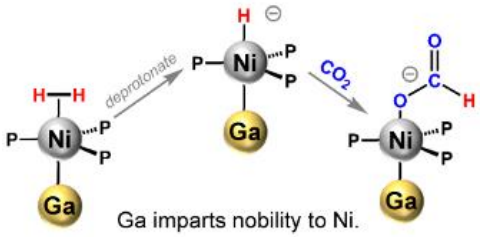
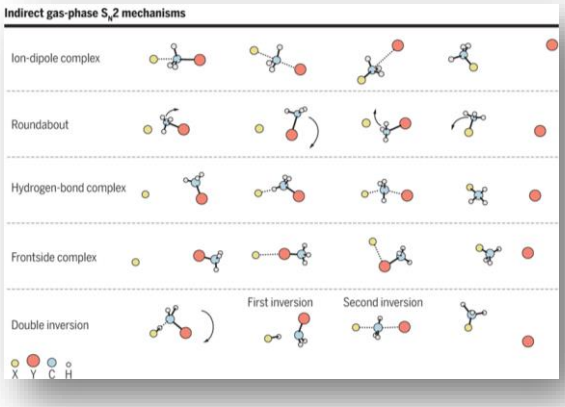
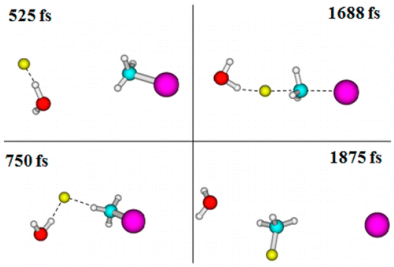
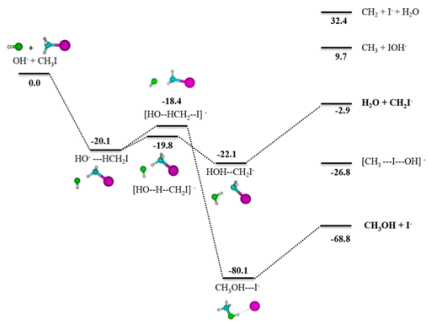
	Featured in the ACS Select virtual issue "JACS Young Investigators," as a highlight of work published by young investigators in JACS in 2017. 
19.	R. C. Cammarota, M. V. Vollmer, **J. Xie**, J. Ye, J. C. Linehan, S. A. Burgess, A. M. Appel, L. Gagliardi, and C. C. Lu.* A Bimetallic Nickel–Gallium Complex Catalyzes CO_2 Hydrogenation via the Intermediacy of an Anionic d^{10} Nickel Hydride, ***J. Am. Chem. Soc.***, **2017**, 139 (40), 14244–14250 
18.	N. H. Anderson, **J. Xie**, D. Ray, M. Zeller, L. Gagliardi, S. C. Bart.* Elucidating Bonding Preferences in Tetrakis(imido)uranate(VI) Dianions. ***Nat. Chem.*** **2017**, 9, 850–855
17.	**J. Xie**, X. Ma, J. Zhang, P. M. Hierl, A. A. Viggiano, W. L. Hase.* Effect of Microsolvation on the $OH^-(H_2O)_n$ + CH_3I Rate Constant. Comparison of Experiment and Calculations for $OH^-(H_2O)_2$ + CH_3I. *Int. J. Mass. Spectrom.* **2017**, 418, 122-129
16.	X. Liu, **J. Xie**, L. Yang,* J. Zhang,* W. L. Hase. Steric Effects of Solvent Molecules on S_N2 Substitution Dynamics. *J. Phys. Chem. Lett.*, **2017**, 8.8, 1885-1892
15.	S. Pratihar, X. Ma, **J. Xie**, R. Scott, E. Gao, B. Ruscic, A. J. A. Aquino, D. W. Setser, W. L. Hase.* Post-transition state dynamics and product energy partitioning following thermal excitation of the F···HCH_2CN transition state: Disagreement with experiment. *J. Chem. Phys.* **2017**, 147, 144301
14.	L. Yang, X. Liu, J. Zhang,* **J.Xie**. Effect of microsolvation on a S_N2 reaction. Indirect atomistic dynamics and weakened suppression of reactivity. Phys. *Chem. Chem. Phys.* ***2017***, 19.15, 9992-9999
13.	L. Yang, J. Zhang,* **J. Xie**, C. Zhao. Competing E2 and S_N2 Mechanisms for the F^- + CH_3CH_2I Reaction. *J. Phys. Chem. A.* **2017**, 121 (5), 1078–1085
12.	**J. Xie**, W. L. Hase.* Rethinking the S_N2 reaction. ***Science,*** **2016**, 6281 (352), 32-3

	
11.	J. Zhang, L. Yang,* **J. Xie**, W. L. Hase. Microsolvated $F^-(H_2O)$ + CH_3I S_N2 Reaction Dynamics. Insight into the Suppressed Formation of Solvated Products. *J. Phys. Chem. Lett.*, **2016**, *7* (4), 660–665 
10.	**J. Xie**, R. Otto, R. Wester, W. L. Hase.* Chemical dynamics simulations of the monohydrated $OH^-(H_2O)$ + CH_3I reaction. Atomic-level mechanisms and comparison with experiment. *J. Chem. Phys*. **2015**, *142*, 244308
9.	**J. Xie**, M. McClellan, R. Sun, S. C. Kohale, N. Govind, W. L. Hase.* Direct Dynamics Simulation of Dissociation of the $[CH_3$--I--$OH]^-$ Ion-Molecule Complex. *J. Phys. Chem. A* ***2015,*** *119,* 817-825
8.	**J. Xie**, J. Zhang, W. L. Hase.* Is There Hydrogen Bonding for Gas Phase S_N2 Pre-Reaction complexes? *Int. J. Mass. Spectrom.* **2015**, *378,* 14-19
7.	**J. Xie**, Scott, M. J., Hase,* W. L., Hierl, P. M., Viggiano, A. A. Determination of the Temperature-Dependent $OH^-(H_2O)$ + CH_3I Rate Constant by Experiment and Simulation. *Zeitschrift für Physikalische Chemie*, **2015**, *229*(10-12), 1747-1763
6.	J. Zhang, **J. Xie**, W. L. Hase.* Dynamics of the F^-+ CH_3I→ HF+ CH_2I^- Proton Transfer Reaction. *J. Phys. Chem. A*, **2015,***119*(50), 12517-12525
5.	R. Sun, **J. Xie**, J. Zhang, W. L. Hase.* The F^- + CH_3I → FCH_3 + I^- Entrance Channel Potential Energy Surface. Comparison of Electronic Structure Methods. *Int. J. Mass. Spectrom.* **2015**, *377,* 222-227
4.	**J. Xie**, R. Otto, J. Mikosch, J. Zhang, R. Wester, W. L. Hase.* Identification of Atomic-Level Mechanisms for Gas-Phase X^- + CH_3Y S_N2 Reactions by Combined Experiments and Simulations. ***Acc. Chem. Res.*** **2014,** 47, 2960-2969

	
3.	**J. Xie**, S. C. Kohale, W. L. Hase,* S. G. Ard, J. J. Melko, N. S. Shuaman, A. A. Viggiano, Temperature Dependence of the OH^- + CH_3I Reaction Kinetics. Experimental and Simulation. *J. Phys. Chem. A*, **2013**, *117,*14019–14027
2.	**J. Xie**, R. Sun, M. R. Siebert, R. Otto, R. Wester, W. L. Hase.* Direct Dynamics Simulations of the Product Channels and Atomistic Mechanisms for the OH^- + CH_3I Reaction. Comparison with Experiment. *J. Phys. Chem. A*, **2013**, *117*, 7162–7178
1.	R. Otto, **J. Xie**, J. Brox, S. Trippel, M. Stei, T. Best, M. R. Siebert, W. L. Hase, R. Wester.* Reaction Dynamics of Temperature-Variable Anion Water Clusters Studied with Crossed Beams and by Direct Dynamics. *Faraday Discuss.* **2012**, *157*, 41-57

教学经历

2020 统计热力学（双语）
2019 物理化学助教
2017 Honor’s 普通化学助理讲师
2014, 2013 有机化学助理讲师
2014, 2013 物理化学助理讲师
2011 普通化学实验助