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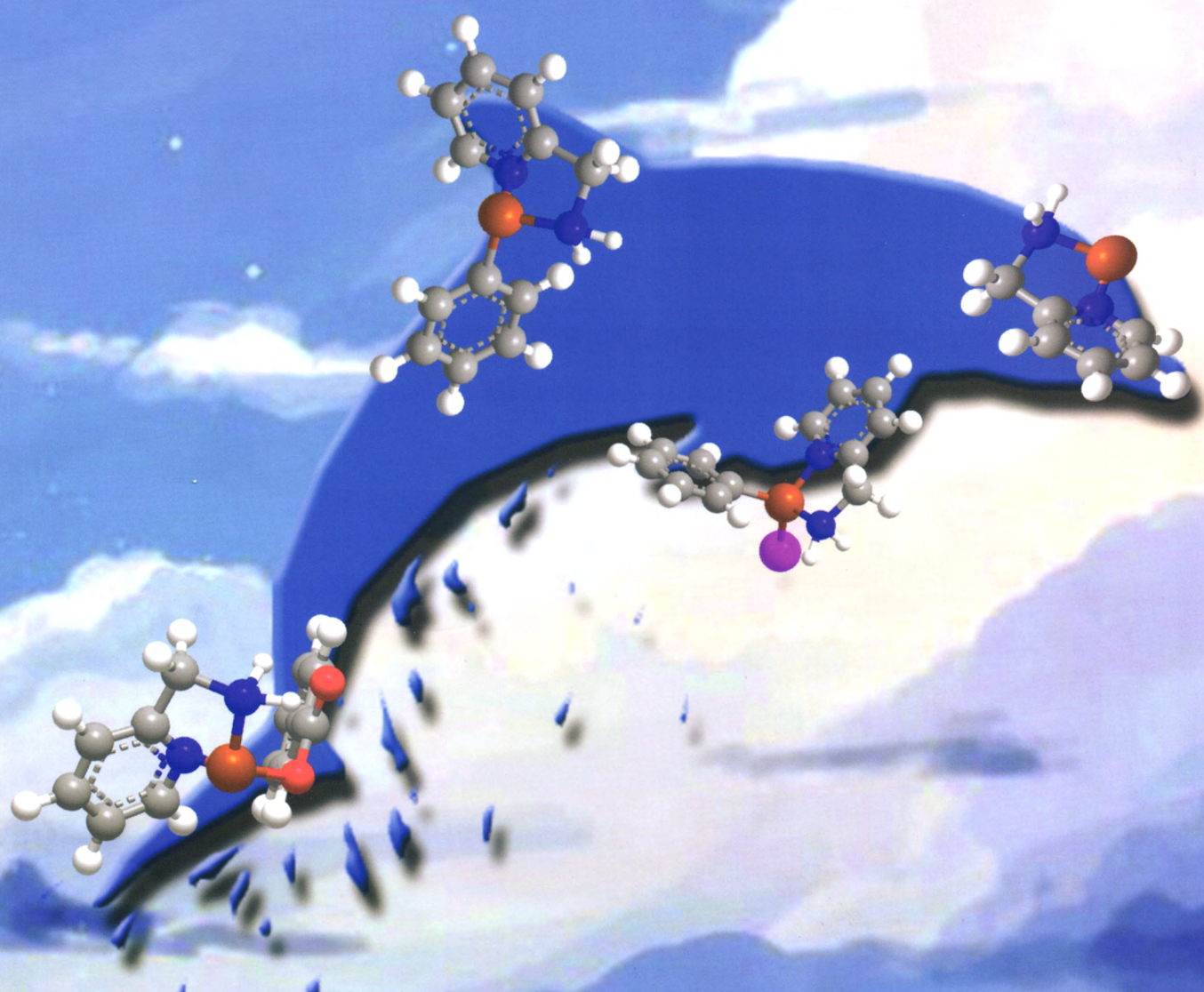
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主办

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(Huaxue Xuebao)

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目 次

综述

溶剂型智能驱动材料的研究进展 张大杰, 刘捷, 陈波*, 王京霞*, 江雷, 化学学报, **2018**, 76(6), 425-435

研究通讯

气相中铜催化的脱羧碘化反应 尹欣驰, 江游, 楚士颖, 翁国锋, 方向*, 潘远江*, 化学学报, **2018**, 76(6), 436-439

饱和开链醚的氧化碳氢炔基化研究 关弘浩, 陈磊, 刘磊*, 化学学报, **2018**, 76(6), 440-444

研究论文

硼桥联三氮杂环卡宾配位的铁分子氮配合物: 合成、表征和反应性质研究 凡一明, 程骏, 高亚飞, 施敏*, 邓亮*, 化学学报, **2018**, 76(6), 445-452

高稳定性和水溶性的共轭聚电解质/单壁碳纳米管复合物的制备和表征 朱明晶, 彭娟*, 唐萍, 邱枫, 化学学报, **2018**, 76(6), 453-459

基于碳量子点的稳定高效全色随机激光 郝梓帆, 袁方龙, 王子飞, 李淑花, 范楼珍*, 化学学报, **2018**, 76(6), 460-466

石墨毡载纳米 $\delta\text{-MnO}_2$ 高性能除铵净水材料研究 孙梦佳, 吴天怡, 李天玉, 郭凤巧, 唐阳, 莫恒亮, 杨志涛, 万平玉*, 化学学报, **2018**, 76(6), 467-474

实验与理论研究 G-四链体中鸟嘌呤自由基阳离子脱质子反应 王英辉, 节家龙, 赵红梅, 白羽, 秦佩萱, 宋迪*, 化学学报, **2018**, 76(6), 475-482

限域单分子层冰-水两相平衡体系的分子动力学模拟 杜涵, 梁洪涛, 杨洋*, 化学学报, **2018**, 76(6), 483-490

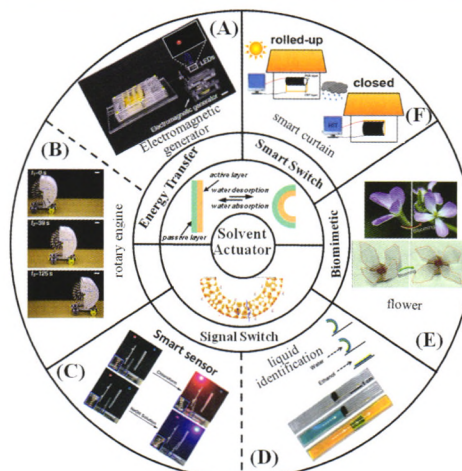
* 通信联系人.

On the cover: Organocopper complexes were synthesized in the electrospray ionization mass spectrometry. Gas phase decarboxylative iodination reactions were carried out by collision-induced dissociation and ion-molecule reactions. During these processes, the valence state change of copper was observed, and the mechanism of copper-catalyzed decarboxylative iodination was examined. [Pan, Yuanjiang *et al.* on page 436-439.]



Review

Research Progress of Solvent-based Smart Actuator Materials



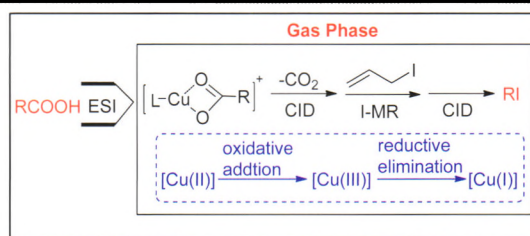
Zhang, Dajie; Liu, Jie; Chen, Bo*; Wang, Jingxia*; Jiang, Lei

Acta Chim. Sinica **2018**, 76(6), 425-435

The concept, fabrication approach and the relative applications of solvent-responsive actuating materials are reviewed, it is of significance for the development of novel actuator devices.

Communication

Copper-Catalyzed Decarboxylative Iodination Reaction in the Gas Phase

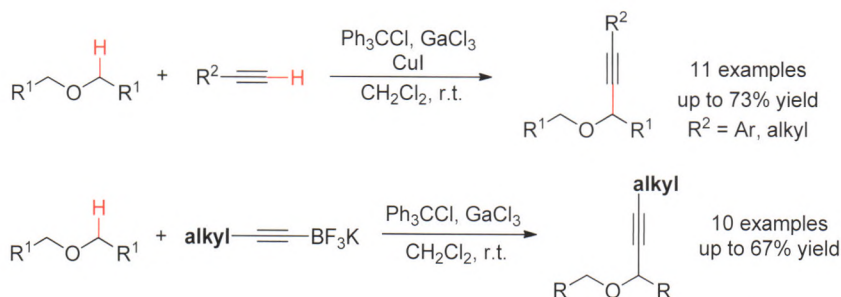


Yin, Xinch; Jiang, You; Chu, Shiyang; Weng, Guofeng; Fang, Xiang*; Pan, Yuanjiang*

Acta Chim. Sinica **2018**, 76(6), 436-439

Carboxylic acid was introduced to electrospray ionization mass spectrometry in methanol with Cu^{2+} and bidentate nitrogen ligand to generate the Cu(II) complex ion in the gas phase. With collision-induced dissociation and ion-molecule reaction with allyl iodide, the decarboxylative iodination reaction was carried out to produce iodohydrocarbon. The valence state change of central metal copper was observed.

Oxidative C—H Alkynylation of Unactivated Acyclic Ethers



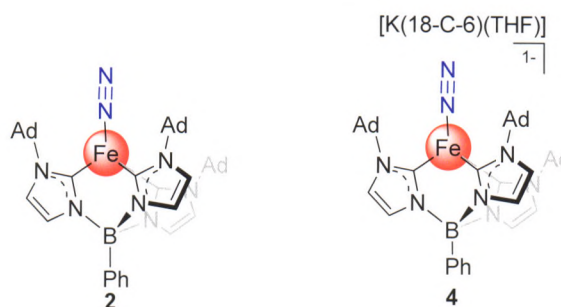
The first cross-dehydrogenative coupling (CDC) of unactivated acyclic ethers and terminal alkynes promoted by Ph₃CCl/GaCl₃ is reported. The mild reaction proceeded at room temperature in CH₂Cl₂. The Ph₃CCl/GaCl₃ mediated oxidative C—H alkynylation of unactivated acyclic ethers with alkyl substituted alkynylboranes was further established to overcome the relative low efficiency for the CDC reaction involving alkyl substituted terminal alkynes.

Guan, Honghao; Chen, Lei; Liu, Lei*

Acta Chim. Sinica **2018**, 76(6), 440-444

Article

Iron Dinitrogen Complexes Supported by Tris(NHC)borate Ligand: Synthesis, Characterization, and Reactivity Study

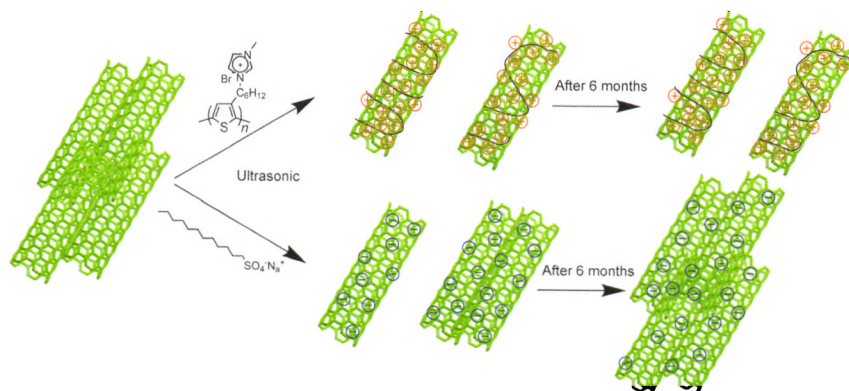


Fan, Yiming; Cheng, Jun; Gao, Yafei; Shi, Min*; Deng, Liang*

Acta Chim. Sinica **2018**, 76(6), 445-452

N₂ activation: the high-spin tetrahedral iron(I)- and iron(0)-N₂ complexes **2** and **4** based on tris(NHC)borate ligand were prepared, which can catalyze the reductive silylation of N₂ by KC₈ and ClSiMe₃ to afford N(SiMe₃)₃ with TON up to 87.

Preparation and Characterization of Highly Stable and Aqueous Dispersion of Conjugated Polyelectrolyte/Single-Walled Carbon Nanotube Nanocomposites

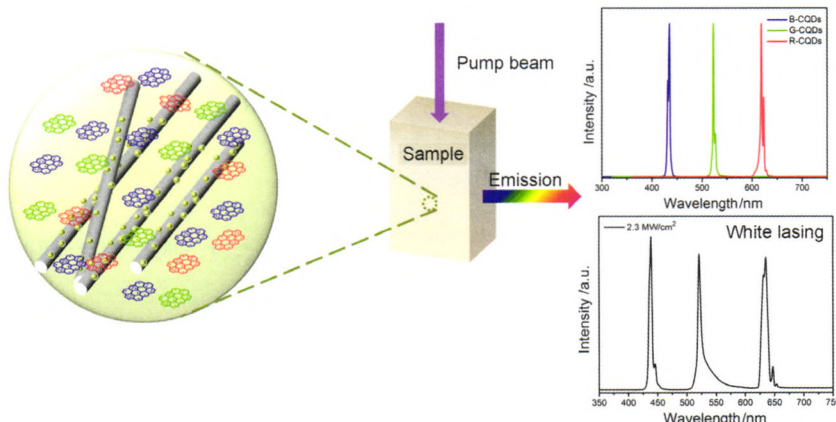


Poly[3-[6-(*N*-methylimidazolium)-hexyl]thiophene] (P3MHT) was designed and used to disperse SWNTs through non-covalent strategy. The P3MHT backbones were wrapped around individual SWNTs via π - π interactions to form the charge-transfer complexes. The ionic side chains of P3MHT not only made the nanocomposites dispersed in water, but also prevented the aggregation of SWNTs by electrostatic repulsion, resulting in aqueous dispersion of P3MHT/SWNTs nanocomposites. Such P3MHT/SWNTs nanocomposite solution exhibited high stability which remained almost unchanged after 6 months while SDS/SWNTs nanocomposite had already precipitated then.

Zhu, Mingjing; Peng, Juan*; Tang, Ping; Qiu, Feng

Acta Chim. Sinica **2018**, 76(6), 453-459

Highly Efficient and Stable Full-Color Random Lasing Emission Based on Carbon Quantum Dots

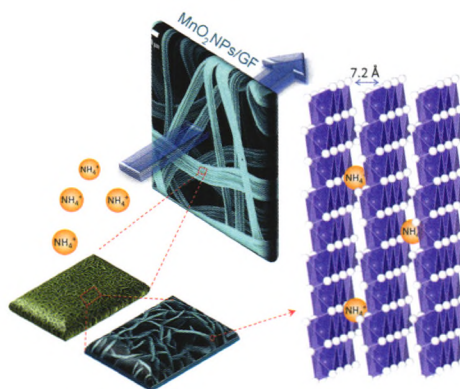


Xi, Zifan; Yuan, Fanglong; Wang, Zifei; Li, Shuhua; Fan, Louzhen*

Acta Chim. Sinica **2018**, 76(6), 460-466

The monochrome CQDs-based random lasing with low excitation threshold have been realized by using Au-Ag bimetallic porous nanowires as scatterers for the first time. Furthermore, white lasing was first demonstrated by combining red, green, blue fluorescent CQDs.

Research on High Performance Ammonium Removal Materials Based on δ -MnO₂ Nanoplate Arrays Decorated Graphite Felt

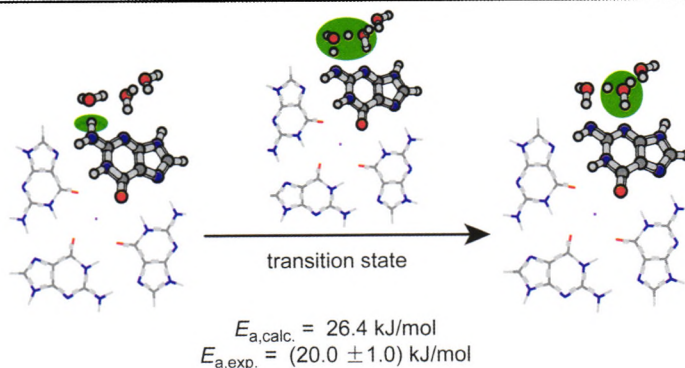


Sun, Mengjia; Wu, Tianyi; Li, Tianyu; Guo, Fengqiao; Tang, Yang; Mo, Hengliang; Yang, Zhitao; Wan, Pingyu*

Acta Chim. Sinica **2018**, 76(6), 467-474

Composite material with hierarchical structure of ultra-thin δ -MnO₂ nanoplate arrays decorated 3D graphite felt (MnO₂NPs/GF) was prepared by a facile *in-situ* redox reaction of KMnO₄ solution and GF. The 7.2 Å interlayer spacing of δ -MnO₂ and the vertical growth of interlaced δ -MnO₂ nanoplate arrays on the GF, prompt MnO₂NPs/GF as a competent candidate material for ultrafast removal of NH₄⁺.

Deprotonation of Guanine Radical Cation in G-Quadruplex: A Combined Experimental and Theoretical Study



Wang, Yinghui; Jie, Jialong; Zhao, Hongmei; Bai, Yu; Qin, Peixuan; Song, Di*

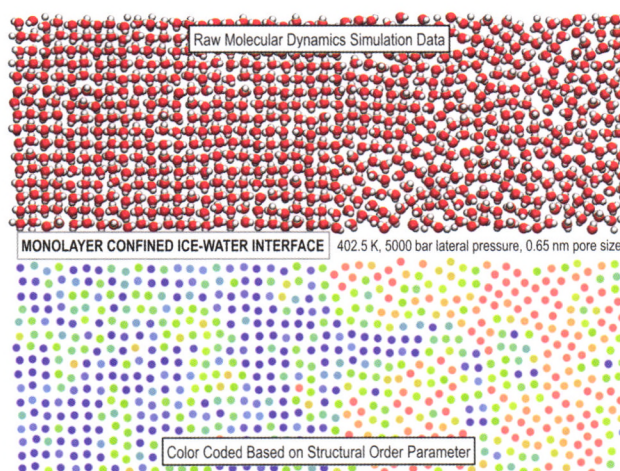
Acta Chim. Sinica **2018**, 76(6), 475-482

The G^{•+} deprotonation in G-quadruplex AG₃(T₂AG₃)₃ has been investigated experimentally and theoretically. The time-resolved absorption spectra and formation kinetics of deprotonation product are measured at different temperatures, from which deprotonation activation energy is determined to be 20.0 ± 1.0 kJ/mol. By carefully considering hydration environment of G^{•+} deprotonation in the G-quadruplex, the potential energy profile for this process is calculated at the M062X/6-31G(d) level. The calculated energy barrier of 26.4 kJ/mol matches with the measured value.

Molecular Dynamics Simulation of Monolayer Confined Ice-Water Phase Equilibrium

Du, Han; Liang, Hongtao; Yang, Yang*

Acta Chim. Sinica **2018**, 76(6), 483-490



A methodology for studying the coexistences of two confined phases of water, based on equilibrium molecular-dynamics (MD) simulations, is presented. The methodology is applied to the coexistence of the monolayer ice and water (described with a simple water model) confined in the 0.65 nm size pore under a lateral pressure of 5000 bar, yielding a direct determination of the melting point and extensive atomic-scale characterization for the mono-molecular layer containing the confined ice-water coexistence line.

《化学学报》2018年编辑委员会全体会议成功召开暨 “《化学学报》2016年度最有影响力论文奖”揭晓

5月4日晚,“《化学学报》2018年编辑委员会全体会议”在杭州召开。《化学学报》主编:周其林;副主编:丁奎岭、孙世刚、田禾、赵宇亮;以及陈军等72位编委老师出席了会议。优秀论文奖作者曾毅、任旻等,《化学学报》编辑部杨侠、潘冰峰、丁卫锋、孙贺平等也参加了会议。

会议首先由周其林主编致辞,对新老编委表示感谢,感谢大家一直以来对《化学学报》的支持和贡献,同时也对《化学学报》近年取得的进步表示了肯定。《化学学报》主管杨侠博士向各位主编、副主编和编委老师们介绍了《化学学报》的历史,汇报了从2012年下半年改版以来的工作进展情况,以及取得的成绩和存在的问题。接下来各位老师相继发言,对期刊的发展建言献策并进行了热烈的讨论。

此次编委会议总结了上一届编委会的工作情况,完成了编委的换届工作,强调了办好中文期刊历史使命和重大意义,确立了“促进中国化学、传承中国文化”的办刊宗旨,制定了期刊发展的新目标,并讨论了提高期刊学术质量、影响力的措施和办法、期刊宣传的重要性及策略、提高编委活跃度的措施,通过了组建编委会微信群、开设《化学学报》研究生论坛等决议,为《化学学报》今后的发展指明了方向。

会议期间还进行了“《化学学报》2016年最有影响力论文奖”颁奖典礼,江海龙、叶轩立、朱晨等作者的9篇文章分别获奖(见封三),周其林、丁奎岭、孙世刚、田禾、赵宇亮分别向获奖作者颁奖并合影留念。

