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中国科学院上海有机化学研究所

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(Huaxue Xuebao)

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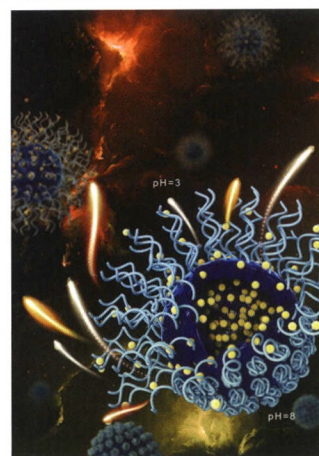
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研究论文

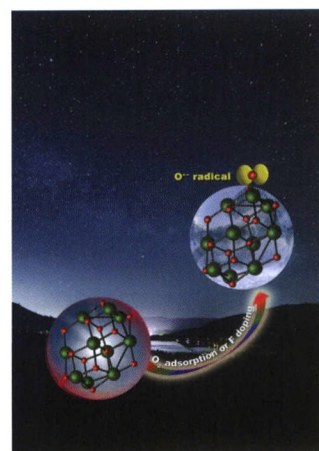
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- 纳米尺寸氧化钪团簇阴离子与正丁烷反应的研究 阮曼, 赵艳霞*, 何圣贵*, 化学学报, 2021, 79(4), 490-499
- pH 敏感型智能高分子单链力学性能研究 于淼, 赵武, 张凯, 郭鑫*, 化学学报, 2021, 79(4), 500-505
- 液相合成彩色氮化碳及其光电化学特性研究 何利蓉, 唐笑*, 张灵, 李艳虹, 相国涛, 周贤菊, 凌发令, 姚璐, 蒋浩, 化学学报, 2021, 79(4), 506-512
- $CuO/CeO_2-ZrO_2/SiC$ 整体催化剂催化甲醇水蒸气重整制氢的研究 焦桐, 许雪莲, 张磊*, 翁幼云, 翁玉冰, 高志贤, 化学学报, 2021, 79(4), 513-519
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- 分级结构碳纳米笼高效催化苄胺氧化偶联制 N -苄烯丁胺 曾誉, 吕品, 蔡跃进, 高福杰, 卓欧, 吴强*, 杨立军, 王喜章*, 胡征, 化学学报, 2021, 79(4), 539-544

* 通信联系人.

On the cover: Single-molecule force spectroscopy experiments show that the pH-sensitive polymer undergoes a conformational change from random coil to collapse with pH changes. Based on this property, the conceptual design of molecular motors and molecular switches is proposed, which provides theoretical support for the design and development of smart polymer sensors. [Xin Guo *et al.* on page 500-505.]

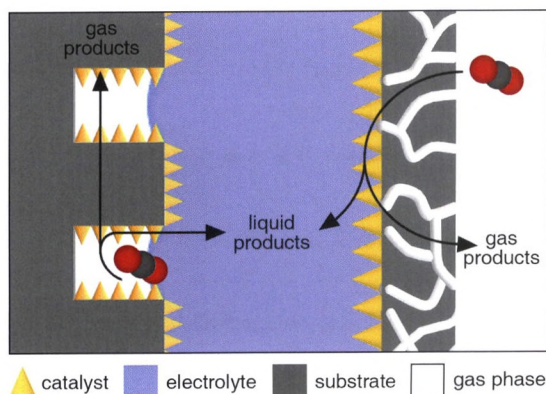


On the back cover: The adsorption of O_2 or F onto unreactive metal oxide clusters results in the generation of $O^{\cdot-}$ radicals, which reveals new mechanisms of the formation of $O^{\cdot-}$ radicals on metal oxide surfaces and provides new insights into the design of novel transition metal oxide-based catalysts. [Yan-Xia Zhao *et al.* on page 490-499.]



Review

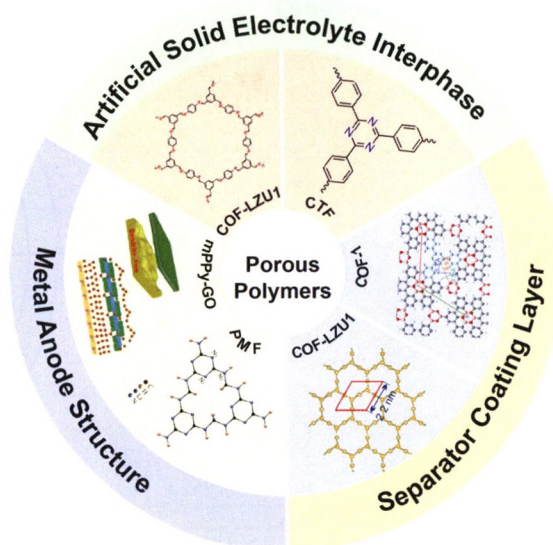
Research Progress on Triphase Interface Electrocatalytic Carbon Dioxide Reduction



In this review, the classification and principle of triphase electrocatalytic systems are discussed, and the influence of wettability and interfacial diffusion on triphase electrocatalytic systems is further explored. Finally, the existing problems in the field of triphase electrocatalytic carbon dioxide reduction are put forward and the future development is prospected.

Yining Ma, Run Shi*, Tierui Zhang*
Acta Chim. Sinica **2021**, 79(4), 369-377

Recent Progress of Porous Polymers for Lithium Metal Anodes Protection

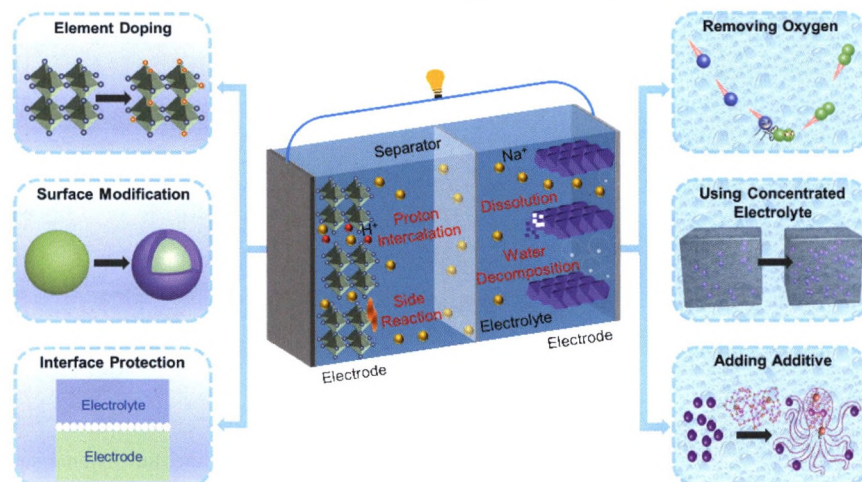


Rong Zhuang, Xiaosa Xu, Changzhen Qu, Shunqi Xu, Tao Yu, Hongqiang Wang*, Fei Xu*

Acta Chim. Sinica **2021**, 79(4), 378-387

Li metal is a promising anode, but uncontrollable dendrite growth still remains challenging for Li metal batteries. The recent progress of designing porous polymers as the artificial solid electrolyte interphase layer, functional layers coated on separators and host for constructing anode structure, aiming to elimination of Li dendrites is summarized in this review.

Research Progress and Practical Challenges of Aqueous Sodium-Ion Batteries



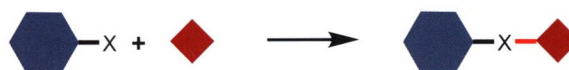
Hui Ma, Huanrong Zhang, Mianqi Xue*

Acta Chim. Sinica **2021**, 79(4), 388-405

The latest developments in electrode material, electrolyte and current collector of aqueous sodium-ion batteries, as well as the application challenges and corresponding strategies to develop high-performance aqueous sodium-ion batteries are mainly summarized in this review. Finally, the development prospects of aqueous sodium-ion batteries are discussed.

Recent Progress of Bioorthogonal Chemistry in China

Bioorthogonal Ligation Reaction



Bioorthogonal Cleavage Reaction

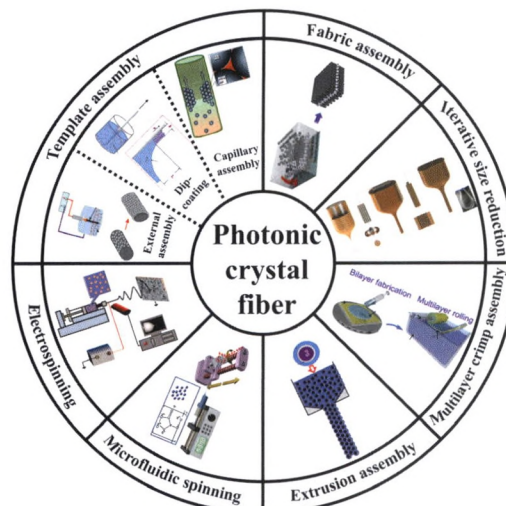


Xin Wang, Xianrui Zhang, Zongyu Huang, Xinyuan Fan*, Peng R. Chen*

Acta Chim. Sinica **2021**, 79(4), 406-413

Bioorthogonal chemistry has become powerful tools for biological studies, which consists of bioorthogonal ligation reaction and bioorthogonal cleavage reaction.

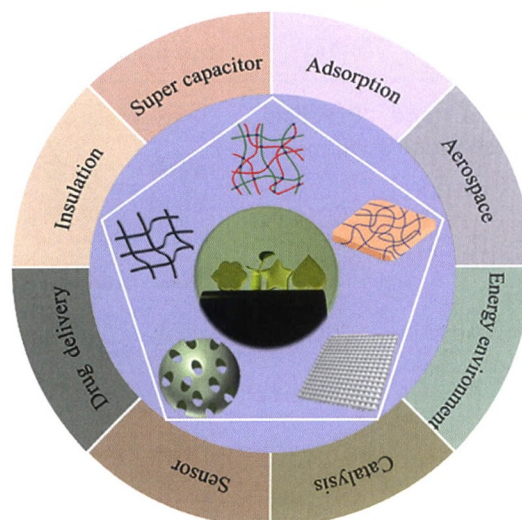
Research Progress of Bioinspired Photonic Crystal Fibers



Guangchen Pei, Jingxia Wang*, Lei Jiang
Acta Chim. Sinica **2021**, 79(4), 414-429

The fabrication, properties and applications of photonic crystal fibers are summarized in this review. It is of great significance for the development of its application in wearable fabrics.

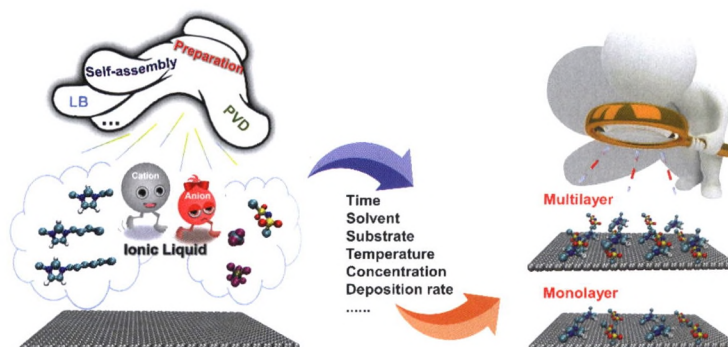
Advances on Dimensional Structure Designs and Functional Applications of Aerogels



Jing Wang, Jin Wang*
Acta Chim. Sinica **2021**, 79(4), 430-442

Recent progress in the dimensional structure designs and functional applications of aerogels are reviewed.

Research Progress on the Preparation and Properties of Two Dimensional Structure of Ionic Liquids



Yumiao Lu, Wei Chen, Yanlei Wang, Feng Huo, Yihui Dong, Li Wei*, Hongyan He*
Acta Chim. Sinica **2021**, 79(4), 443-458

Two-dimensional structure ionic liquids (ILs) can be prepared by self-assembly, Langmuir-Blodgett and physical vapor deposition (PVD) methods. The enhanced surface effect results in unique phase transition feature, mechanical and electrical characteristics of two-dimensional structure ILs, which shows broad potential application prospects in the field of chemistry and materials.

Research Progress in Metal-Organic Framework and Its Composites for Separation of C_2 Based on Sieving Multiple Effects

Xufei Li, Baoyou Yan, Weiqiu Huang*,
Lipei Fu, Xianhang Sun, Aihua Lv

Acta Chim. Sinica **2021**, 79(4), 459-471

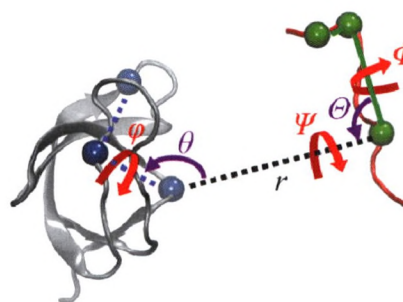


Herein, we concentrate on the sieving metal-organic framework (MOF) and its composites with optimal pore size, Brunauer-Emmett-Teller (BET) surface area and functional groups, which have high efficiency separation of C_2H_2/C_2H_4 and C_2H_4/C_2H_6 .

Accurate Estimation of Protein-ligand Binding Free Energies Based on Geometric Restraints

Haohao Fu, Haochuan Chen, Hong Zhang,
Xueguang Shao*, Wensheng Cai*

Acta Chim. Sinica **2021**, 79(4), 472-480



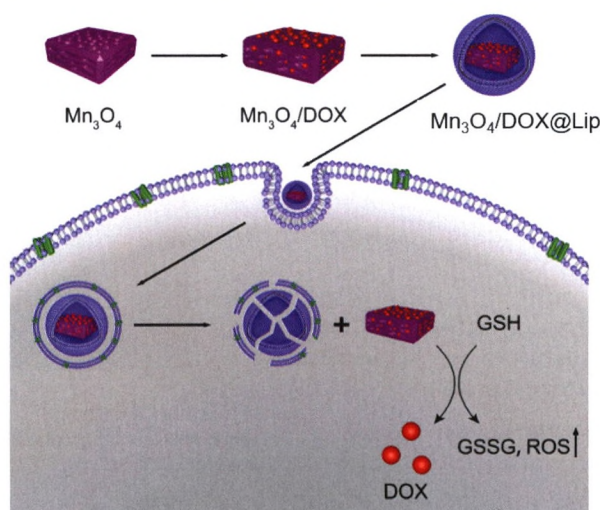
Protein-ligand binding free energies can be accurately estimated using the importance-sampling or alchemical algorithms, providing that the translational, orientational, rotational and conformational restraints are well defined.

Article

The Construction and Application of Mn_3O_4 /DOX@Lip Nano-drug Delivery System Based on Fenton-like Reaction

Zheng Cai, Yingwen Zhang, Liping Jiang*,
Junjie Zhu*

Acta Chim. Sinica **2021**, 79(4), 481-489

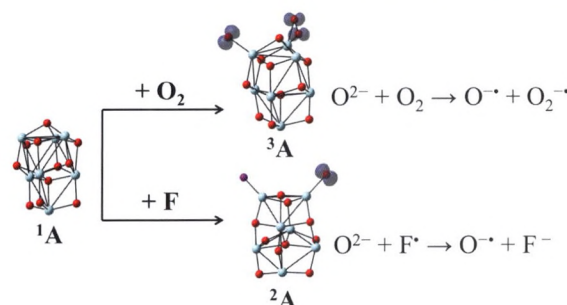


A tumor microenvironment-responsive Mn_3O_4 /DOX@Lip nano-drug delivery system was designed. The nano Mn_3O_4 with uniform morphology was prepared by thermal decomposition. Under low pH and high-level glutathione condition, the drug carrier was broken, releasing Mn^{2+} and anticancer drug (DOX). Mn^{2+} could trigger Fenton-like reaction. With the content of glutathione in the cell was down-regulated, the original oxidation-reduction balance in the cell was destroyed. Oxidative active substance disturbed the cellular oxidative environment and induced cell death. Meanwhile, under oxidative stress conditions, the toxicity of chemotherapy drugs had been enhanced. The proposed Mn_3O_4 /DOX@Lip nano-drug delivery system has a better effect of promoting apoptosis on cancer cells and providing new research strategies for tumor treatment.

Study on the Reaction of Nanosized Yttrium Oxide Cluster Anions with *n*-Butane in the Gas Phase

Man Ruan, Yan-Xia Zhao*, Sheng-Gui He*

Acta Chim. Sinica **2021**, 79(4), 490-499

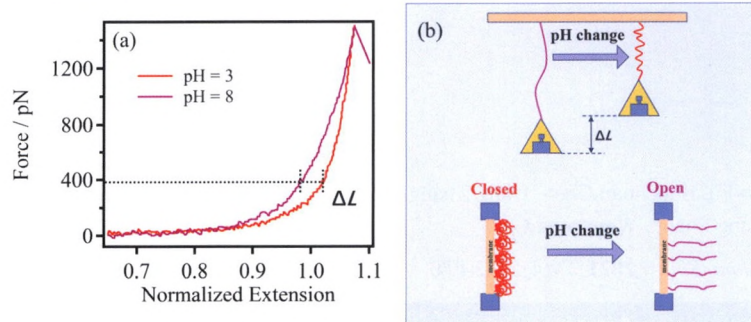


The $O^{\bullet -}$ radicals of $(Y_2O_3)_N YO_4^-$ ($\Delta=4$; $N=1, 3\sim 24$) and $(Y_2O_3)_N YO_2F^-$ ($\Delta=1$; $N=1\sim 24$) can be considered to be generated by the adsorption of an O_2 or F onto the unreactive singlet $(Y_2O_3)_N YO_2^-$ ($\Delta=0$; $N=1\sim 24$) with electron transfer from a oxygen ion (O^{2-}) to the O_2 or F . The studies on gas-phase clusters suggest that adsorption of O_2 or F onto unreactive metal oxide clusters will result in the generation of $O^{\bullet -}$ radical. This work not only reveals the new mechanisms of the formation of $O^{\bullet -}$ radical on metal oxide surfaces, but also provides new insights into the design of novel transition metal oxide-based catalysts.

Single-Molecule Mechanism of pH Sensitive Smart Polymer

Miao Yu, Wu Zhao, Kai Zhang, Xin Guo*

Acta Chim. Sinica **2021**, 79(4), 500-505

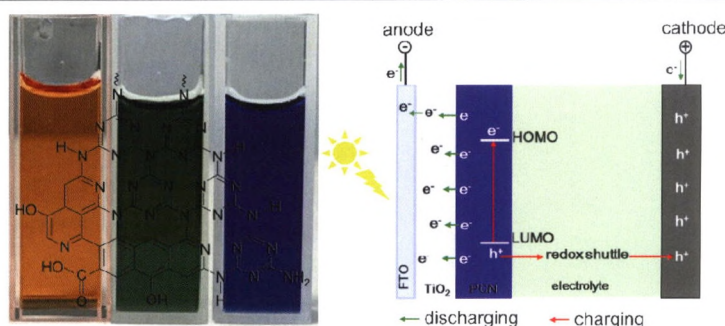


The novel molecular motors (switches) can be proposed according to the variation of single-chain mechanics of pH sensitive polymers.

Study on Photoelectrochemical Properties of Colorful Carbon Nitrides Synthesized in Liquid-Phase

Lirong He, Xiao Tang*, Ling Zhang, Yanhong Li, Guotao Xiang, Xianju Zhou, Faling Ling, Lu Yao, Hao Jiang

Acta Chim. Sinica **2021**, 79(4), 506-512

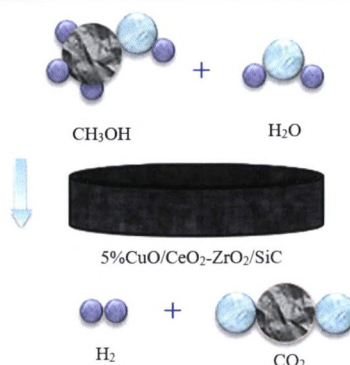


The colorful carbon nitrides synthesized in aqueous solutions demonstrate the intriguing photoelectrochemical property of direct solar-to-electric energy conversion and storage.

Research on CuO/CeO₂-ZrO₂/SiC Monolithic Catalysts for Hydrogen Production by Methanol Steam Reforming

Tong Jiao, Xue-lian Xu, Lei Zhang*, You-yun Weng, Yu-bing Weng, Zhi-xian Gao

Acta Chim. Sinica **2021**, 79(4), 513-519

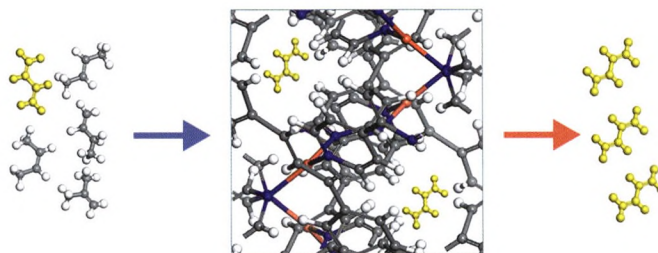


5%CuO/CeO₂-ZrO₂/SiC has relatively higher copper specific surface area, stronger interaction between CuO and support, more oxygen vacancies, thus showing better catalytic activity. Also the SiC support is chemical stable and has favorable thermal conductivity, which avoiding the device volume increase caused by the additional heating device, thus facilitating the integration of minitype reactors for hydrogen generation.

High-throughput Screening of Real Metal-organic Frameworks for Adsorption Separation of C4 Olefins

Lei Yang, Yujing Wu, Xuanjun Wu*, Wei-quan Cai

Acta Chim. Sinica **2021**, 79(4), 520-529

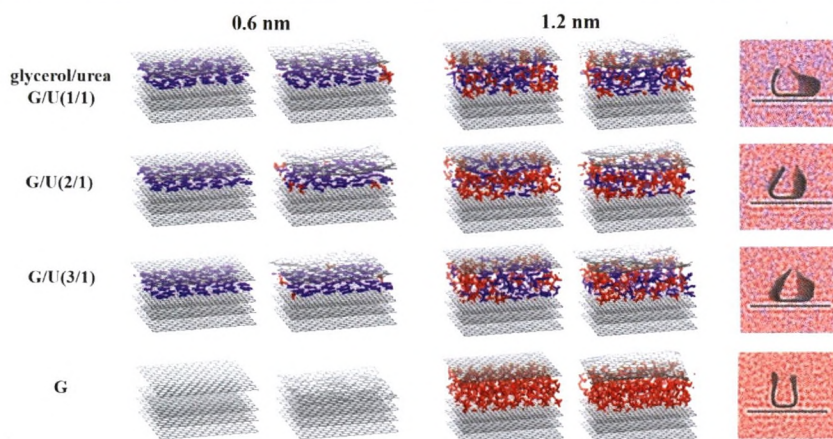


8 MOFs (metal-organic frameworks) with the highest adsorption performance score and structural stability were screened out from 12723 real MOFs using computational high-throughput screening method for C4 olefins separation.

Molecular Dynamics Simulation of the Stability Behavior of Graphene in Glycerol/Urea Solvents in Liquid-Phase Exfoliation

Chang-An Liu, Shi-Bo Hong, Bei Li*

Acta Chim. Sinica **2021**, 79(4), 530-538

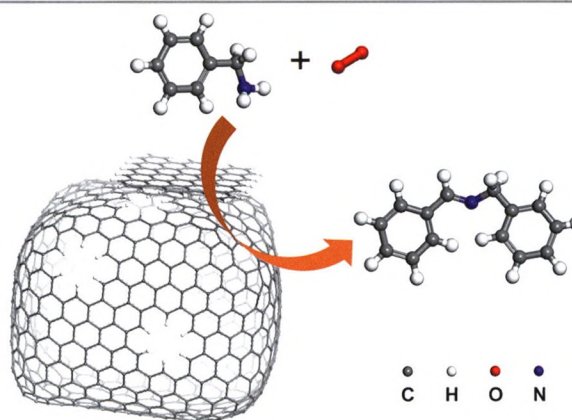


The pristine graphene sheet at an initial interlayer spacing of 0.6 nm in the glycerol solvent restacks back due to the fact that the glycerol molecules fail to diffuse into the graphene interlayer, thereby failing to form a sufficient repulsive barrier to hinder the graphene aggregation. While in other pristine cases, a single- or double-layer solvent structure is formed, offering efficient dispersion medium to stabilize the graphene sheets. Although the pristine graphene sheets present similar stability in different glycerol/urea solvents, the U-type graphene experiences distinct levels of stabilization in solvents in the order of pure glycerol > glycerol/urea(2/1) > glycerol/urea(3/1) > glycerol/urea(1/1), signifying that the exfoliated state of the graphene sheets plays an important role in the stabilization during liquid-phase exfoliation.

Hierarchical Carbon Nanocages as Efficient Catalysts for Oxidative Coupling of Benzylamine to N-Benzylidene Benzylamine

Yu Zeng, Pin Lyu, Yuejin Cai, Fujie Gao, Ou Zhuo, Qiang Wu*, Lijun Yang, Xizhang Wang*, Zheng Hu

Acta Chim. Sinica **2021**, 79(4), 539-544



The hierarchical carbon nanocages prepared at 700 °C exhibits excellent catalytic performance in the solvent-free oxidative coupling of benzylamine to *N*-benzylidene benzylamine under mild conditions (100 °C and atmospheric O₂). Specifically, after reacting for 8 h, both benzylamine conversion and *N*-benzylidene benzylamine selectivity are larger than 98%. Such excellent catalytic performance is mainly ascribed to the abundant defects, unique hierarchical architecture and ultra-high specific surface area.



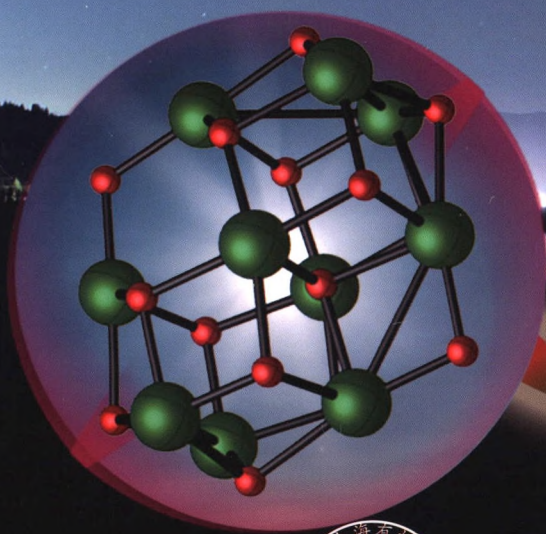
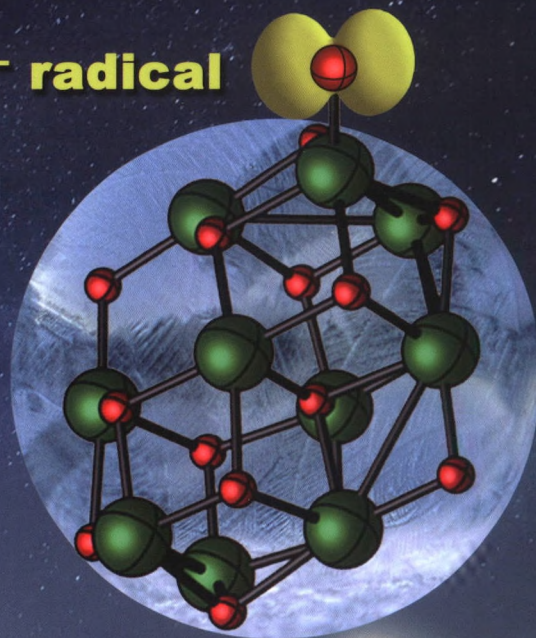
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$\text{O}^{\cdot -}$ radical



O_2 adsorption or F doping



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中国科学院上海有机化学研究所

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