ISSN 0567-7351
CN 31-1320/O6
CODEN HHHPA4
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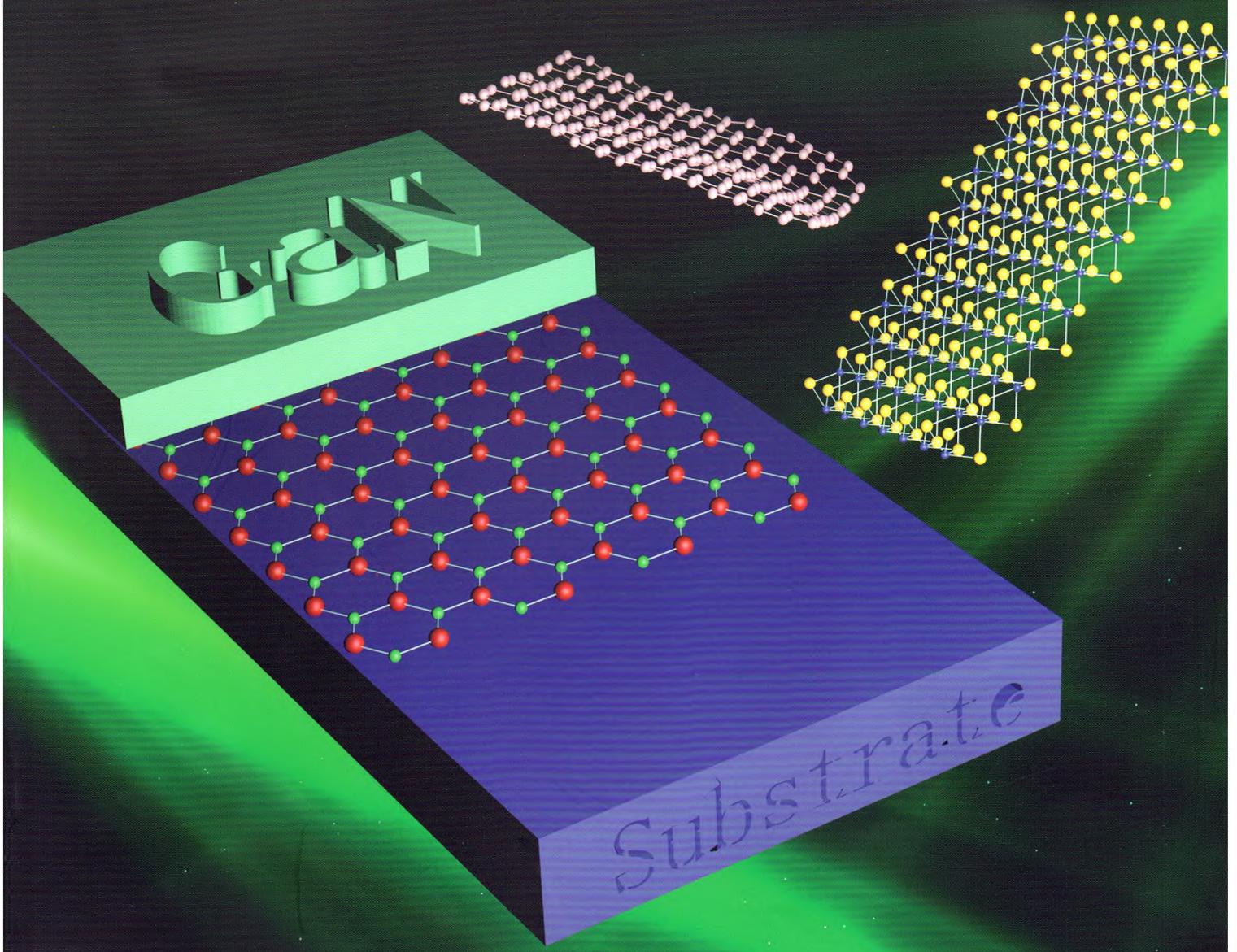
ACTA CHIMICA SINICA

2017 第75卷 第3期 Vol. 75 No. 3



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中国化学会
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化 学 学 报

Acta Chimica Sinica

(Huaxue Xuebao)

第 75 卷　第 3 期　2017 年 3 月 15 日

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ACTA CHIMICA SINICA

Vol. 75, No. 3 March 15, 2017

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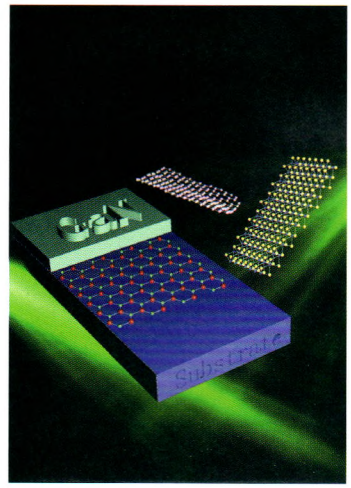


On the cover: Contrary to their bulk counterparts, two-dimensional materials, such as graphene, h-BN and TMDs, are weakly bonded between layers, which can be used in heteroepitaxy of III-Nitrides to reduce the stress caused by large lattice-mismatch. It can also help self-standing fabrication of III-nitrides devices such as InGaN-MQW LED and AlGaN HEMT. [Yang, Shaoyan *et al.* on page 271-279.]

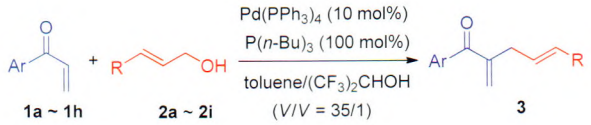
Review

Communication

Morita-Baylis–Hillman Reaction of α,β-Unsaturated Ketones with Allylic Alcohols by the Combination of Transition-Metal Catalysis and Organocatalysis

Li, Yaqiong; Huang, Zhizhen*

Acta Chim. Sinica **2017**, *75*(3), 280-283



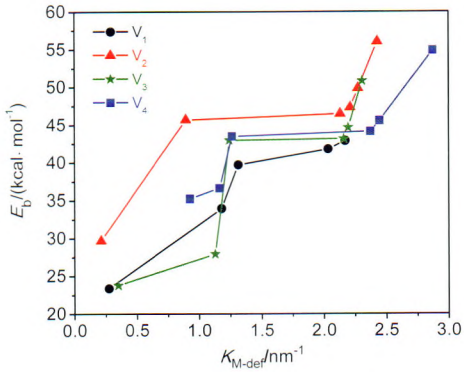
Under the catalysis of $Pd(PPh_3)_4$ and the mediation of $P(n\text{-}Bu)_3$, α,β-unsaturated ketones **1** performs a MBH reaction smoothly with allylic alcohols **2** to give α-allylated products **3** in satisfactory yields.

Article

[1+1] and [2+1] Additions on a (5,5) Single-Walled Carbon Nanotube with $V_1 \sim V_4$ Vacancies Based on Defect Curvature: A First Principles Study

Li, Lei; Jia, Guixiao*; Wang, Xiaoxia; Wu, Tongwei; Song, Xiwen; An, Shengli

Acta Chim. Sinica **2017**, *75*(3), 284-292

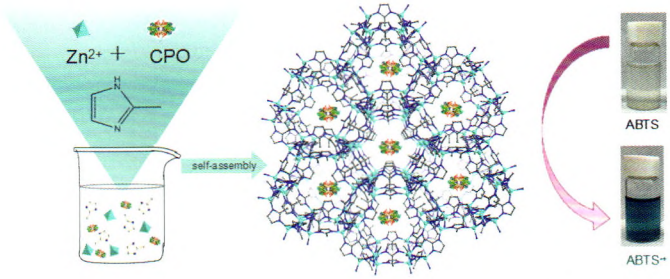


For the atoms at the defect structure area, the binding energies of H atom on the (5,5) tube with $V_1 \sim V_4$ vacancies monotonously increase with the increase of $K_{M\text{-}def}$.

Immobilization of Chloroperoxidase in Metal Organic Framework and Its Catalytic Performance

Zhao, Ruinan; Hu, Mancheng; Li, Shuni; Zhai, Quanguo; Jiang, Yucheng*

Acta Chim. Sinica **2017**, *75*(3), 293-299

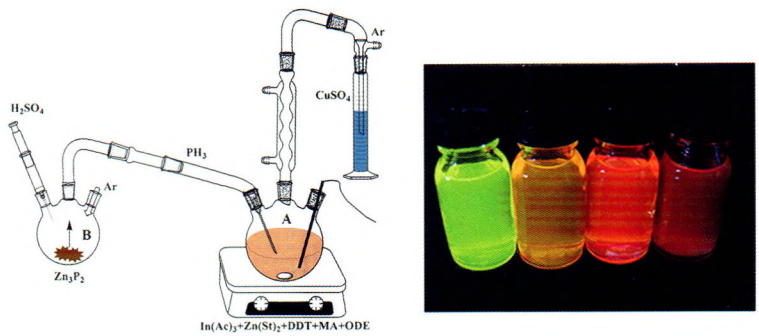


Chloroperoxidase (CPO) was embedded in zeolitic imidazolate frameworks (ZIFs) to prepare CPO@ZIF-8 micro reactor by "one pot" method at 30 ℃ in aqueous solution. The micro reactor displayed high catalytic efficiency to convert ABTS into $ABTS^{\bullet+}$.

Synthesis of InPZnS/ZnS Quantum Dots by Continuous Injection of Phosphorus Precursor

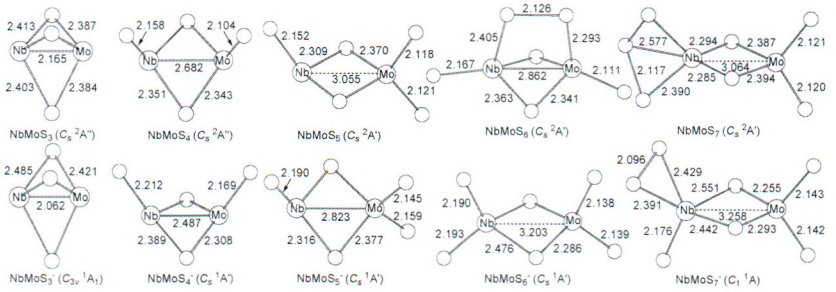
Huang, Lu; Li, Zhichun; Huang, Shouqiang; Peter Reiss; Li, Liang*

Acta Chim. Sinica **2017**, *75*(3), 300-306



The synthetic scheme for the preparation of InPZnS/ZnS QDs based on *in situ* generated gaseous PH_3 from Zn_3P_2. Carried by a flow of Ar gas, PH_3 gas was continuously injected into the indium precursor, resulting in high quality InPZnS/ZnS QDs with emission region from 550 to 680 nm.

Theoretical Investigations on the Structures and the Chemical Bonding of $NbMoS_n^{-/0}$ (n=3~7) Clusters

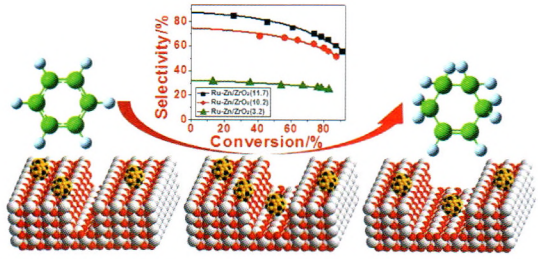


Wang, Bin*; Wang, Jianfu; Zhang, Xiaofei; Chen, Wenjie; Zhang, Yongfan; Huang, Xin

Acta Chim. Sinica **2017**, *75*(3), 307-320

In this work, DFT and CCSD(T) calculations were used to study the $NbMoS_n^{-/0}$ (n=3~7) clusters. $NbMoS_n^{-/0}$ (n=3~7) clusters can be viewed as linking different sulfur ligands to the $NbMoS_2$ four-membered rings. Diverse poly-sulfur ligands emerged in the sulfur-rich clusters. We predicted that doping niobium into the molybdenum sulfides may improve the emergence of S_2 group which may be helpful in producing the coordinatively unsaturated sites (CUS) under the H_2/H_2S atmosphere.

Pore Size Effect of Ru-Zn/ZrO_2 Catalyst on Partial Hydrogenation of Benzene to Cyclohexene



Zhou, Gongbing; Wang, Hao; Pei, Yan; Qiao, Minghua*; Sun, Bin; Zong, Baoning*

Acta Chim. Sinica **2017**, *75*(3), 321-328

The Ru-Zn/ZrO_2 catalysts had a pronounced pore size effect on the selectivity to cyclohexene in the partial hydrogenation of benzene. With the increase in the pore size, the selectivity to cyclohexene increased accordingly. The optimal Ru-Zn/ZrO_2(11.7) catalyst exhibited the highest S_0 (88%) and yield (54%) of cyclohexene.

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