

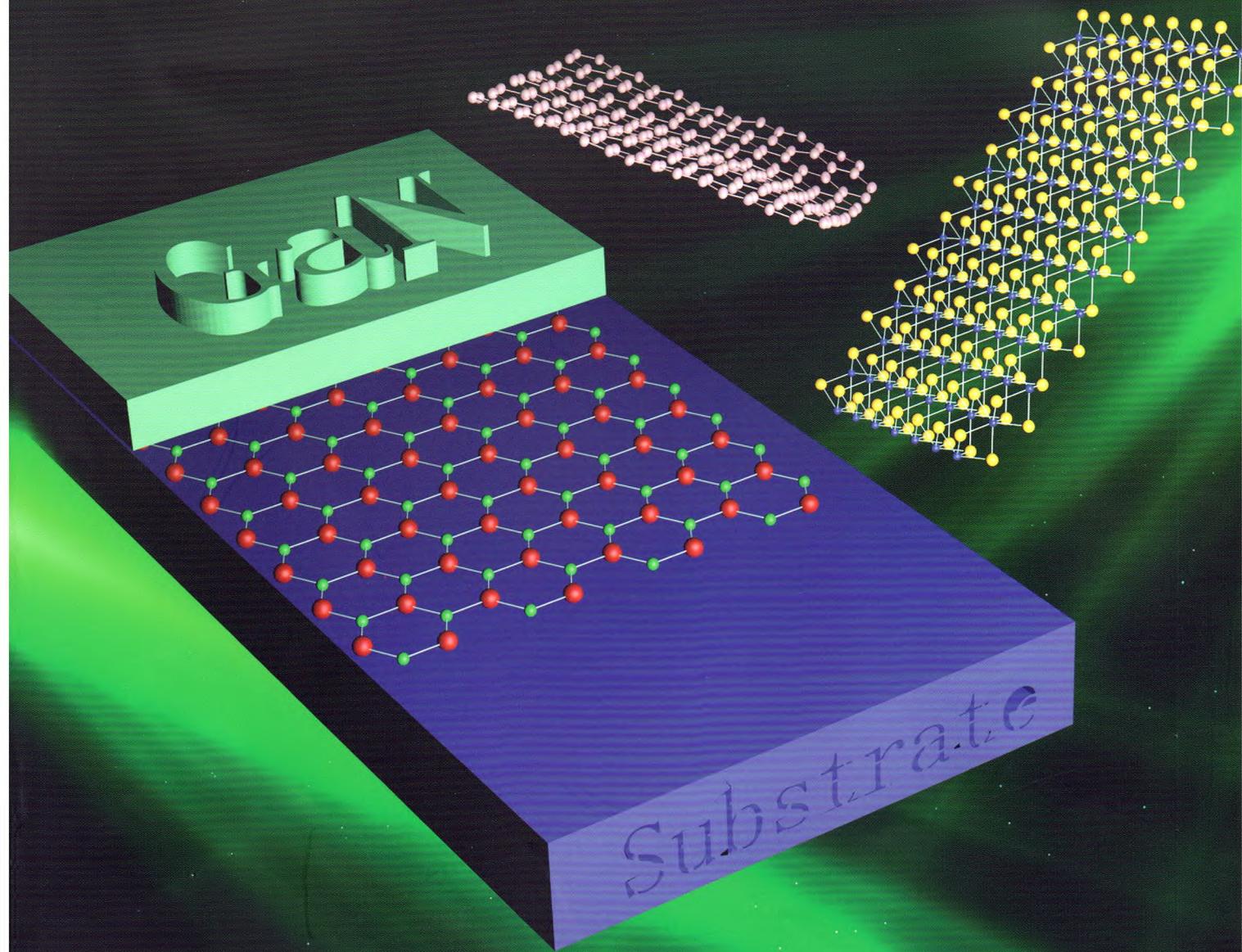


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主办

万方数据

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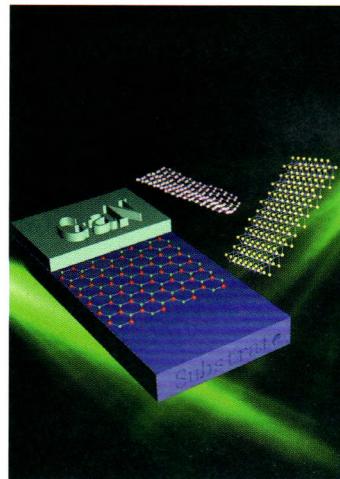
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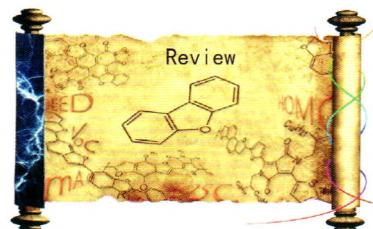
Contents

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

Research Progress of the Furan-Containing Fused Ring Conjugated Organic Molecules and Polymers

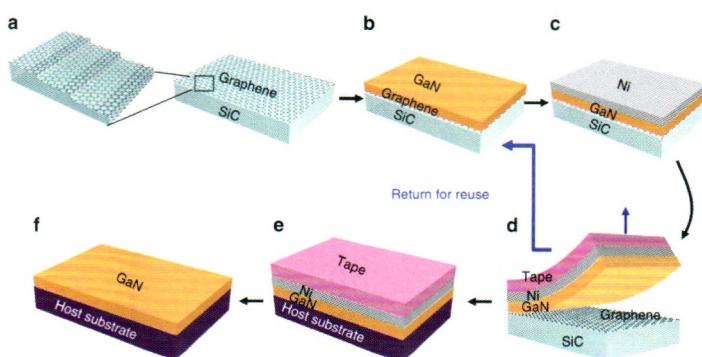


Liu, Ye; Yuan, Jun; Zou, Yingping*; Li, Yongfang

Acta Chim. Sinica 2017, 75(3), 257-270

Furan and furan derivatives possess smaller aromaticity, higher carrier mobility, higher fluorescence quantum efficiency and better solubility. This paper reviewed the recent research progresses of the synthetic methods, properties and applications of the conjugated organic small molecules and polymers based on the furan-containing fused rings.

Epitaxy of III-Nitrides Based on Two-Dimensional Materials



Tan, Xiaoyu; Yang, Shaoyan*; Li, Huijie*

Acta Chim. Sinica 2017, 75(3), 271-279

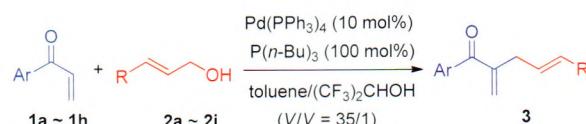
The weak interaction between the 2D materials may facilitate the transfer of III-nitride epitaxial film from its substrate, thus reduces the costs of III-nitride application. Recent achievements on the 2D materials-based epitaxy of III-nitride are reviewed, together with the outlook of its further development. [The picture was reprinted by permission from Macmillan Publishers Ltd: [Nature Communications] (Ref. 37), copyright 2014].

Communication

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

Li, Yaqiong; Huang, Zhizhen*

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



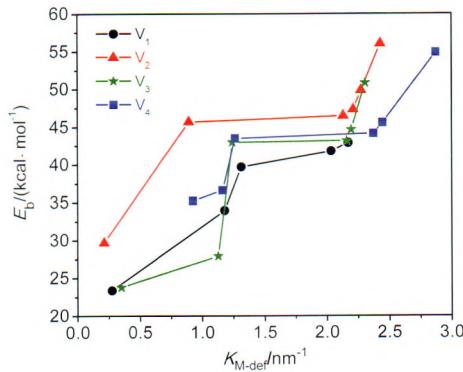
Under the catalysis of $\text{Pd}(\text{PPh}_3)_4$ and the mediation of $\text{P}(n\text{-Bu})_3$, α,β -unsaturated ketones **1** performs a MBH reaction smoothly with allylic alcohols **2** to give α -allylated products **3** in satisfactory yields.

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

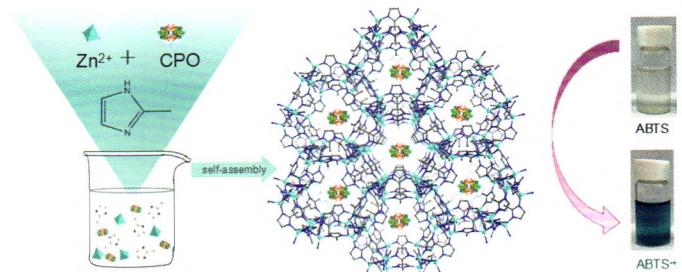


For the atoms at the defect structure area, the binding energies of H atom on the (5,5) tube with $V_1 \sim V_4$ vacancies monotonously increase with the increase of $K_{M\text{-def}}$.

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

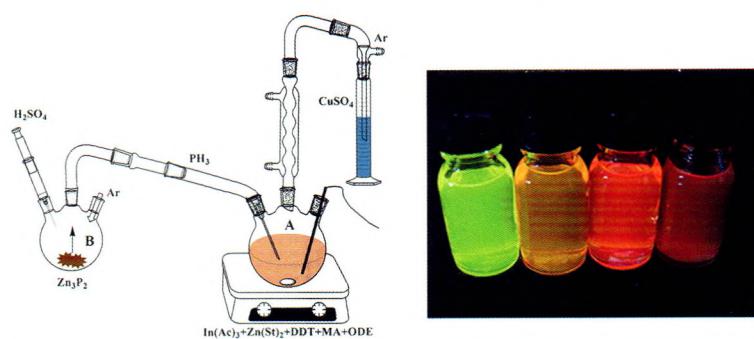


Chloroperoxidase (CPO) was embedded in zeolithic imidazolate frameworks (ZIFs) to prepare CPO@ZIF-8 micro reactor by “one pot” method at 30 °C in aqueous solution. The micro reactor displayed high catalytic efficiency to convert ABTS into ABTS⁺.

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

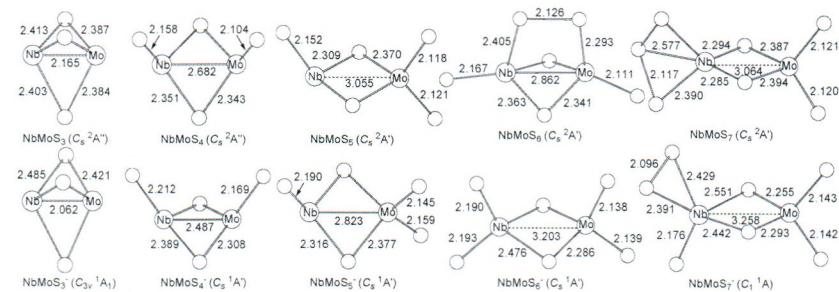
Huang, Lu; Li, Zhichun; Huang, Shouqiang; Peter Reiss; Li, Liang*

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.

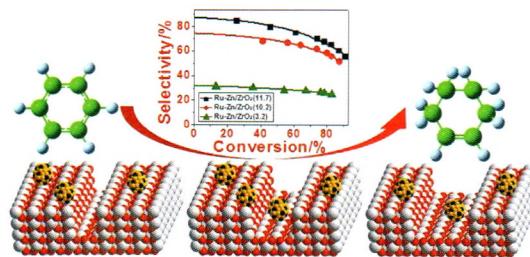
Theoretical Investigations on the Structures and the Chemical Bonding of NbMoS_n^{-10} ($n=3\sim 7$) Clusters



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^{-10} ($n=3\sim 7$) clusters. NbMoS_n^{-10} ($n=3\sim 7$) 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 $\text{H}_2/\text{H}_2\text{S}$ atmosphere.

Pore Size Effect of Ru-Zn/ZrO₂ 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/ZrO₂ 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/ZrO₂(11.7) catalyst exhibited the highest S_0 (88%) and yield (54%) of cyclohexene.



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