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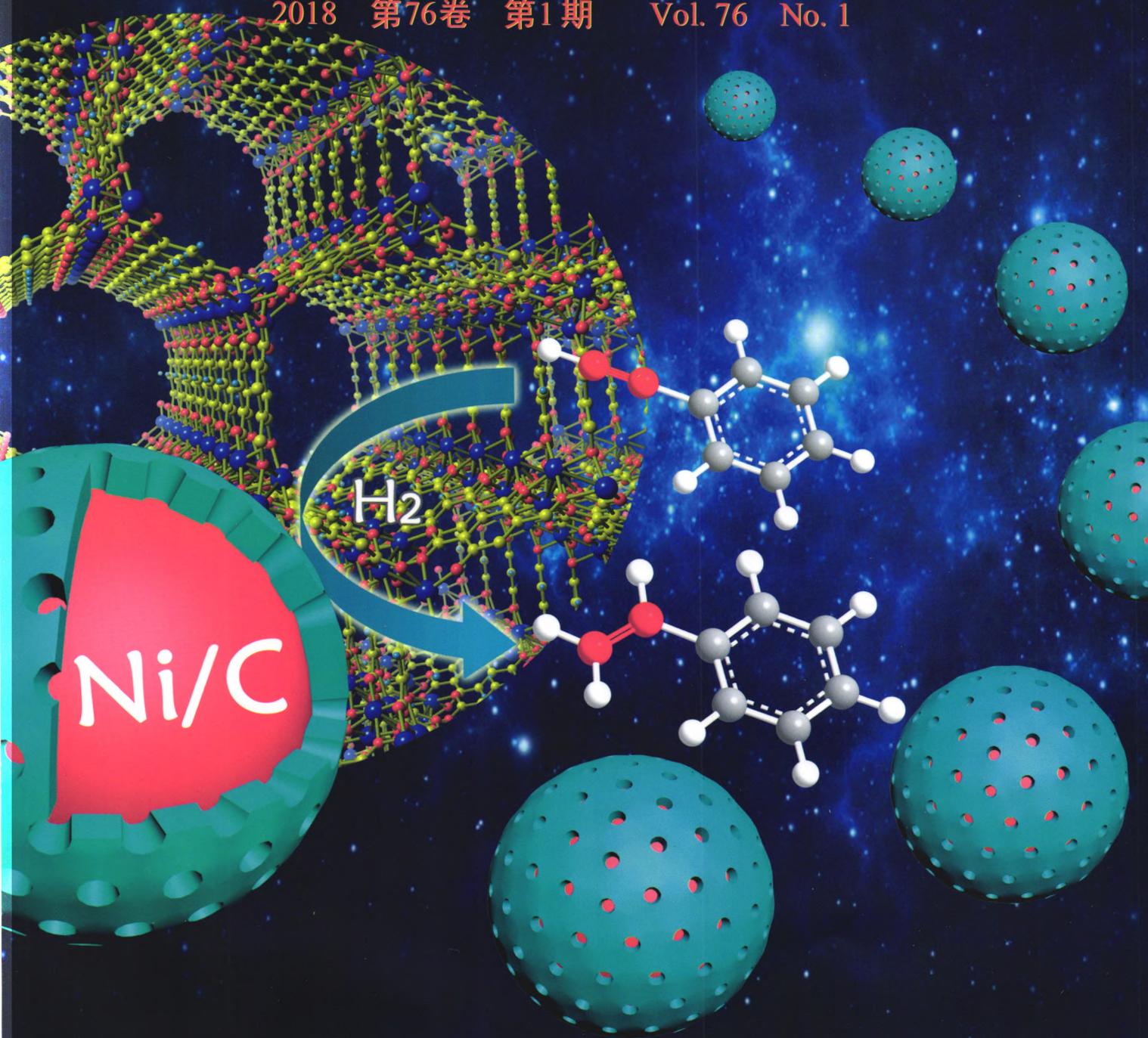


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# 化学学报

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主办

# 化学学报

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(Huaxue Xuebao)

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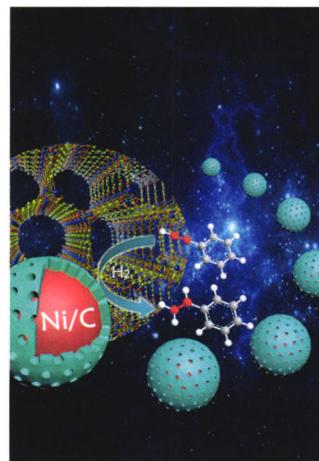
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\* 通信联系人.

## Contents

**On the cover:** A series of Ni/C core-shell nano catalysts with abundant mesoporous and uniform size were prepared by Ni-MOF-74 pyrolysis. The Ni/C exhibits excellent catalytic activity and recyclability in phenylacetylene hydrogenation, which is the most promising transition metal catalyst that can be comparable with noble metal. [Liang, Changhai *et al.* on page 22-29.]

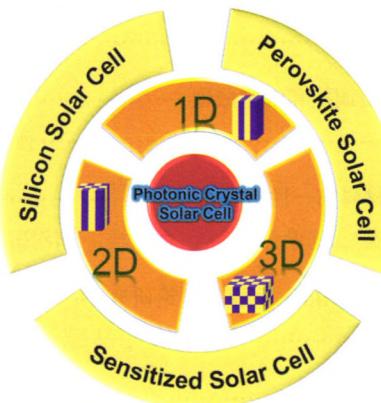


### Review

#### Research Progress of Photonic Crystal Solar Cells

Zhao, Cong; Ma, Ying\*; Wang, Yang; Zhou, Xue; Li, Huizeng; Li, Mingzhu\*; Song, Yanlin

*Acta Chim. Sinica* 2018, 76(1), 9-21



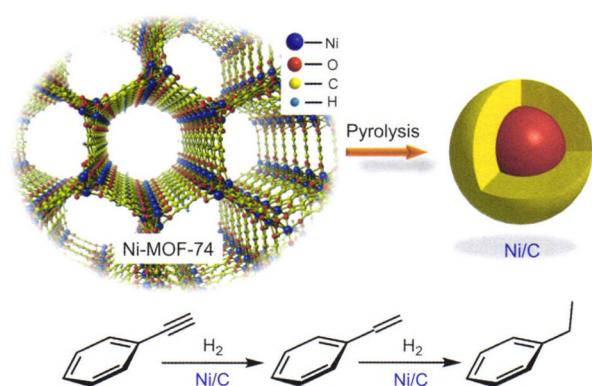
Photonic crystal has shown great potential in solar cells thanks to its unique optical performance including photonic band gap, “slow photon” effect and other unique light control performance. The application of photonic crystals (1D, 2D, 3D) in silicon solar cells, dye-sensitized solar cells and perovskite solar cells are summarized.

### Article

#### Preparation of Ni/C Core-shell Nanoparticles through MOF Pyrolysis for Phenylacetylene Hydrogenation Reaction

Guo, Xiaoling; Chen, Xiao; Su, Dangsheng; Liang, Changhai\*

*Acta Chim. Sinica* 2018, 76(1), 22-29

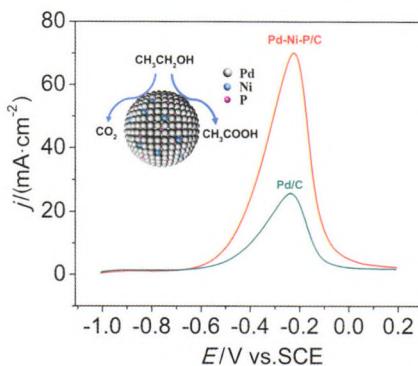


A series of Ni/C Core-shell nano catalysts with rich mesopores were prepared by MOF pyrolysis method and were employed in phenylacetylene (PA) hydrogenation. With an activity of up to  $0.833 \text{ mmol} \cdot \text{min}^{-1} \cdot \text{g}_{\text{cat}}^{-1}$  at  $50^\circ\text{C}$ , Ni/C catalyst exhibited much better catalytic activity than any other reported transition metal catalyst.

**Preliminary Study of Ni and P Low-doped Pd-based Electrocatalysts Toward Ethanol Oxidation Reaction in Alkaline Media**

Zhu, Chan; Hai, Yang; Zhao, Zhigang; Yang, Yaoyue\*

*Acta Chim. Sinica* 2018, 76(1), 30-34

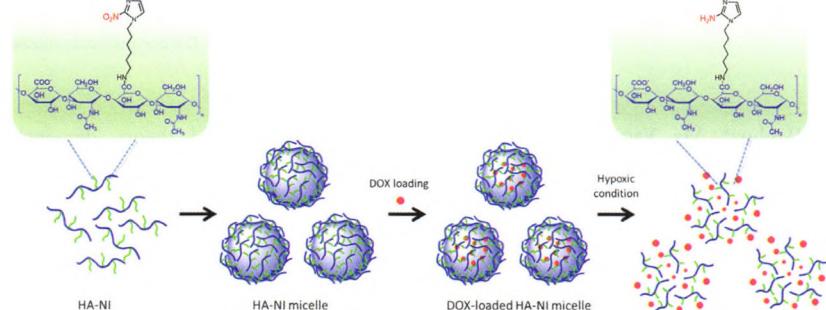


Ni and P low-doped Pd-based electrocatalysts highly increase the catalytic performance of ethanol oxidation in alkaline media. The peak current density of ethanol oxidation on as-prepared Pd-Ni-P/C catalyst is roughly 3 times than that of commercial Pd/C.

**Synthesis and Study of Hypoxia-Responsive Micelles Based on Hyaluronic Acid**

Zhang, Bei; Chang, Baisong; Sun, Taolei\*

*Acta Chim. Sinica* 2018, 76(1), 35-42

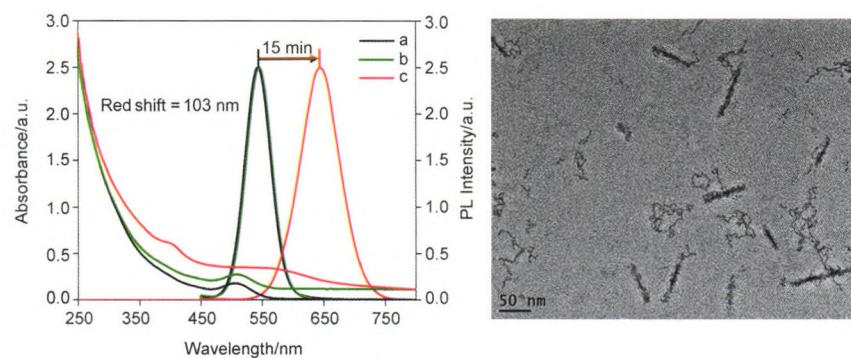


A hypoxia-responsive drug delivery system was developed by grafting hyaluronic acid (HA) with nitroimidazole (NI) derivative. The amphiphilic HA-NI conjugates could self-assemble into micelles and encapsulate doxorubicin (DOX). The micelles generated a much wider size distribution and completely disintegrated under hypoxic condition. *In vitro* drug release studies demonstrated that DOX was released from HA-NI micelles following a hypoxia-dependent manner.

**$(\text{NH}_4)_2\text{MoS}_4$ -Guided Self-Assembly of CdTe QDs and Control over Their Optical Properties and Cell Imaging**

Sun, Quanhong; Li, Zhi; Ma, Nan\*

*Acta Chim. Sinica* 2018, 76(1), 43-48

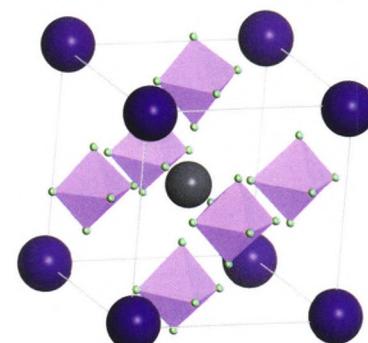


$(\text{NH}_4)_2\text{MoS}_4$ -guided self-assembly of CdTe QDs is a simple and quick method to adjust the emission wavelength of CdTe QDs. By this method, emission wavelength of CdTe QDs underwent a red-shift of more than 100 nm for 15 min at 100 °C in the presence of  $(\text{NH}_4)_2\text{MoS}_4$ .

**Superhalogen Substitutions in Cubic Halide Perovskite Materials for Solar Cells: A First-principles Investigation**

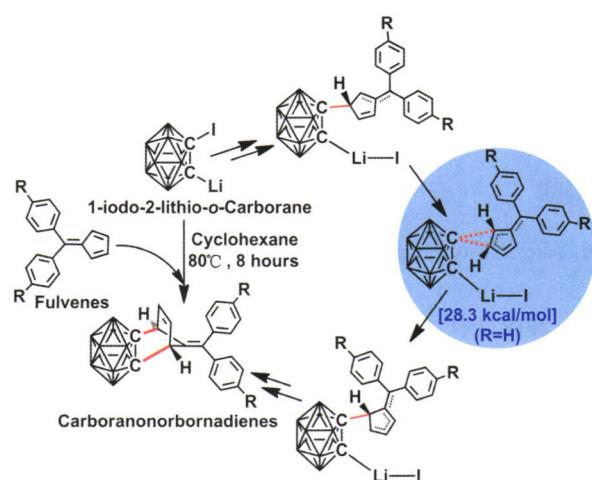
Wu, Miao Miao\*; Liu, Shiqiang; Chen, Hao; Wei, Xuehu; Li, Mingyang; Yang, Zhibin\*; Ma, Xiangdong

*Acta Chim. Sinica* 2018, 76(1), 49-54



We designed a series of new perovskite materials through substituting  $\text{I}^-$  anions in  $\text{CsPbI}_3$  by superhalogen clusters and studied their structures and properties in first-principles way. It is demonstrated that  $\text{CsPb}(\text{PCl}_6)_3$ 's bandgap is 1.58 eV and could be a potential candidate material for solar cells.

**Computational Insights into the Diels-Alder-alike Reactions of 1-Iodo-2-Lithio-o-Carborane with Fulvenes**

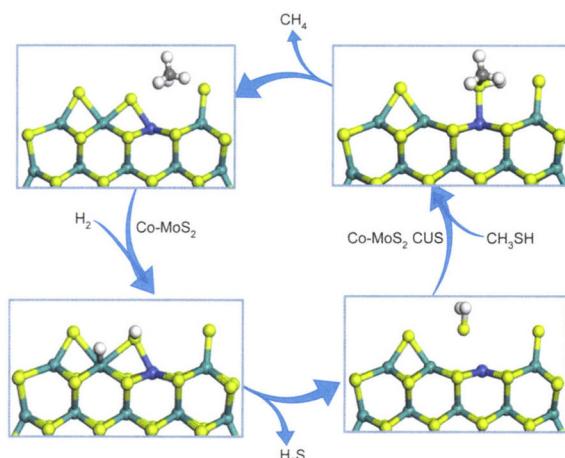


Mu, Weihua\*; Ma, Yao; Fang, Decai; Wang, Rong; Zhang, Haina

*Acta Chim. Sinica* 2018, 76(1), 55-61

Density functional theory demonstrates a stepwise formation mechanism of carboranonorbornadienes from 1-iodo-2-lithio-o-carborane and fulvenes. The IDSCRF-B3LYP/DZVP level results predict consistent half-lives and rates with corresponding experimental yield under given reaction conditions.

**Investigation on CH<sub>3</sub>SH Desulfurization Mechanism at the Edge Site of Co-Doped MoS<sub>2</sub> Cluster**



Zhang, Tian; Guo, Chen; Wei, Shuxian; Wu, Zhonghua; Han, Zhaoxiang; Lu, Xiaoqing\*

*Acta Chim. Sinica* 2018, 76(1), 62-67

The complete desulfurization process includes the formation of CUS and the desulfurization process of CH<sub>3</sub>SH. The formation of CUS starts with H<sub>2</sub> dissociation followed by H<sub>2</sub>S generation and desorption. CH<sub>3</sub>SH adsorbed at the CUS site, followed by the bonds scissions thus the removal of S and CH<sub>4</sub> formation.



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