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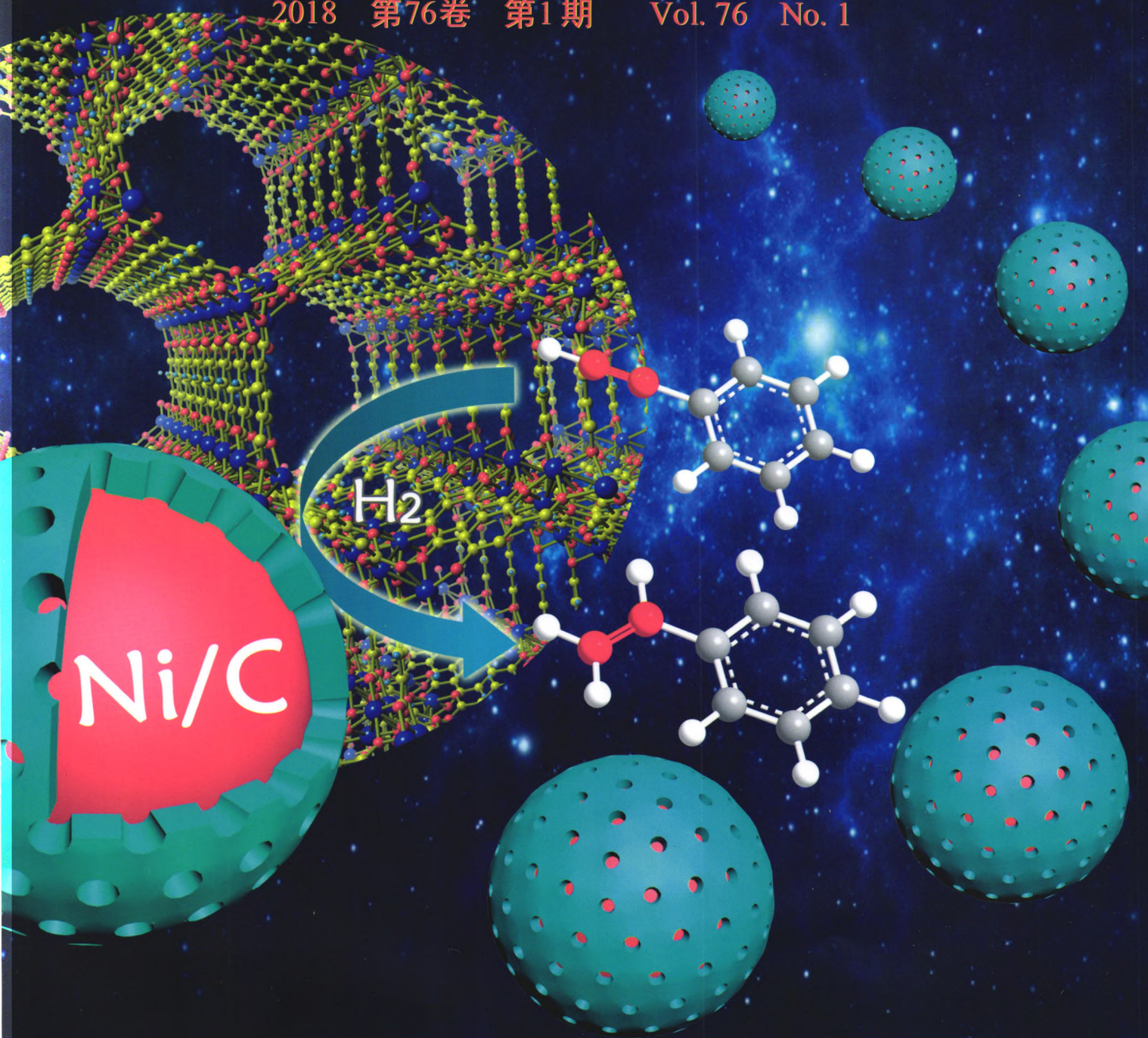

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(Huaxue Xuebao)

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研究论文

* 通信联系人.

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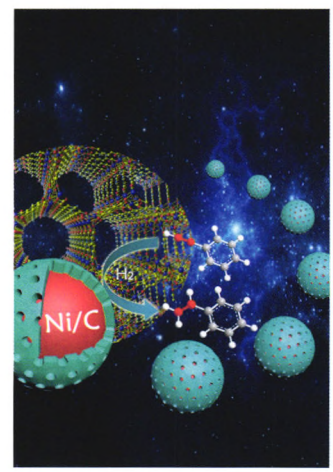

On the cover: A series of Ni/C core-shell nano catalysts with abundant mesoporous and uniform size were prepared by Ni-MOF-74 pyrolysis. The Ni/C exhibits excellent catalytic activity and recyclability in phenylacetylene hydrogenation, which is the most promising transition metal catalyst that can be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

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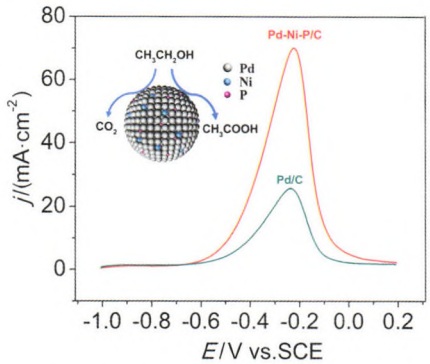
Preliminary Study of Ni and P Low-doped Pd-based Electrocatalysts Toward Ethanol Oxidation Reaction in Alkaline Media

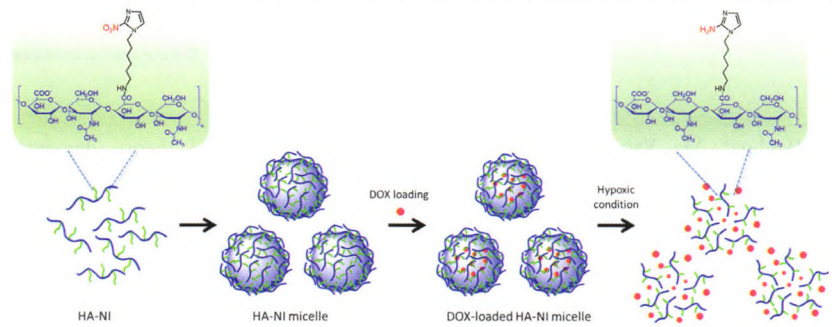


Ni and P low-doped Pd-based electrocatalysts highly increase the catalytic performance of ethanol oxidation in alkaline media. The peak current density of ethanol oxidation on as-prepared Pd-Ni-P/C catalyst is roughly 3 times than that of commercial Pd/C.

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

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

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

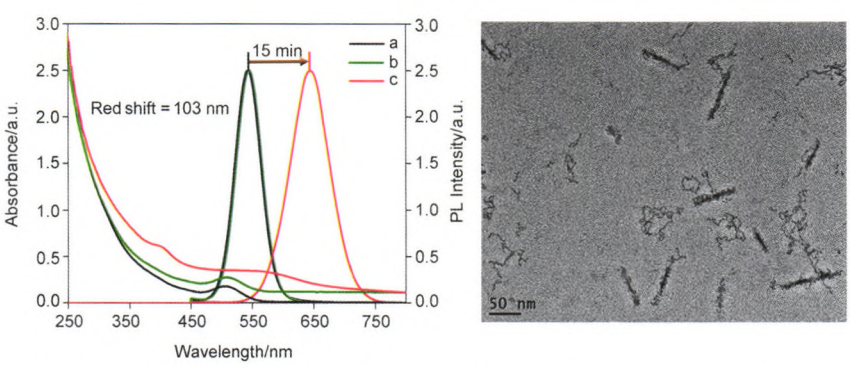


A hypoxia-responsive drug delivery system was developed by grafting hyaluronic acid (HA) with nitroimidazole (NI) derivative. The amphiphilic HA-NI conjugates could self-assemble into micelles and encapsulate doxorubicin (DOX). The micelles generated a much wider size distribution and completely disintegrated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

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

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

$(NH_4)_2MoS_4$-Guided Self-Assembly of CdTe QDs and Control over Their Optical Properties and Cell Imaging

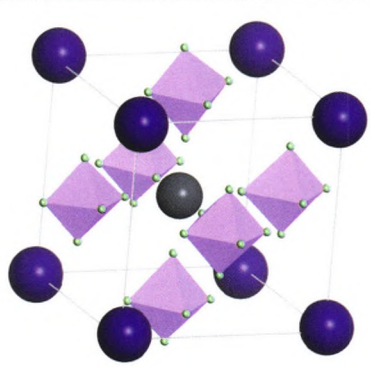


$(NH_4)_2MoS_4$-guided self-assembly of CdTe QDs is a simple and quick method to adjust the emission wavelength of CdTe QDs. By this method, emission wavelength of CdTe QDs underwent a red-shift of more than 100 nm for 15 min at 100 ℃ in the presence of $(NH_4)_2MoS_4$.

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

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

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



We designed a series of new perovskite materials through substituting I^- anions in $CsPbI_3$ by superhalogen clusters and studied their structures and properties in first-principles way. It is demonstrated that $CsPb(PCl_6)_3$'s bandgap is 1.58 eV and could be a potential candidate material for solar cells.

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

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

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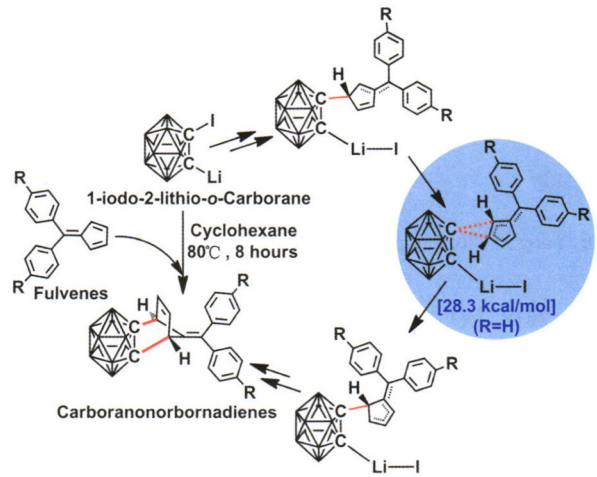
Computational Insights into the Diels-Alder-alike Reactions of 1-Iodo-2-Lithio-*o*-Carborane with Fulvenes

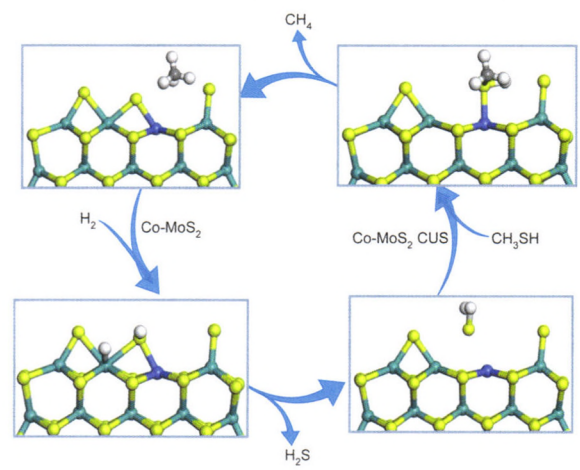


Mu, Weihua*; Ma, Yao; Fang, Decai; Wang, Rong; Zhang, Haina

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-lifes and rates with corresponding experimental yield under given reaction conditions.

Investigation on CH_3SH Desulfurization Mechanism at the Edge Site of Co-Doped MoS_2 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_3SH. The formation of CUS starts with H_2 dissociation followed by H_2S generation and desorption. CH_3SH adsorpted at the CUS site, followed by the bonds scissions thus the removal of S and CH_4 formation.

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