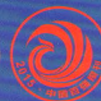


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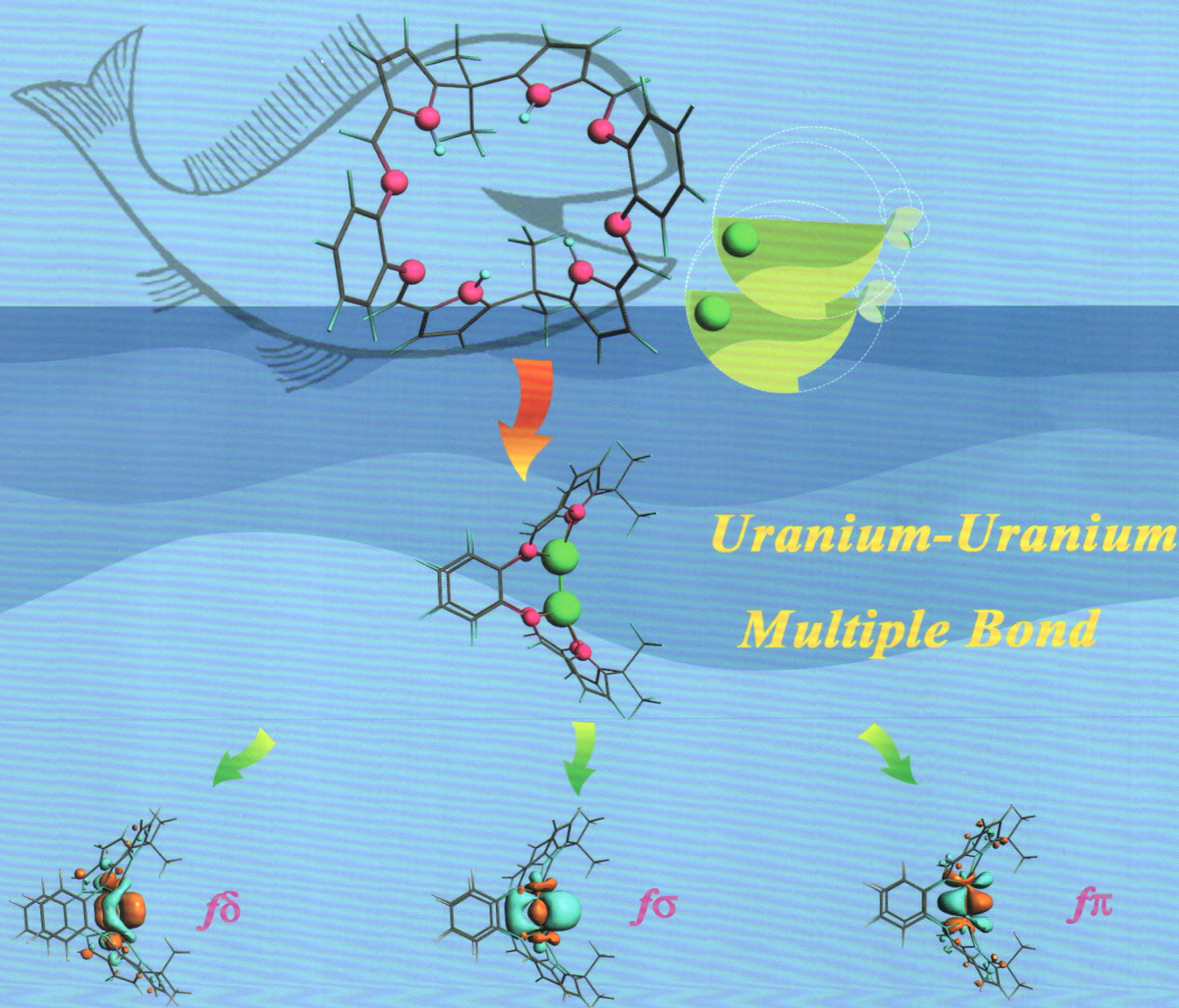


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# 化学学报

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主办



# 化学学报

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## 目次

### 研究展望

- 金催化去芳构化反应研究进展 ..... 吴文挺, 张立明\*, 游书力\*, 化学学报, 2017, 75(5), 419-438

### 综述

- 金属氧化物催化生物质衍生羧酸酮基化研究进展 ..... 丁爽, 葛庆峰, 祝新利\*, 化学学报, 2017, 75(5), 439-447

### 研究通讯

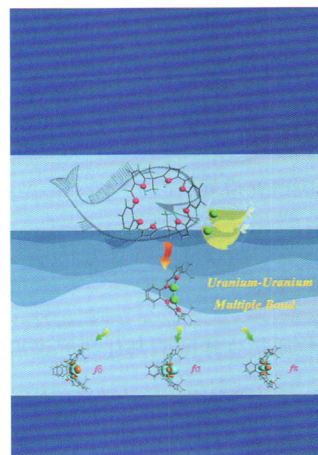
- 钪/氨基酸共催化环己酮分子内  $\alpha$ -烯基化反应 ..... 李保乐, 刘人荣, 梁仁校, 贾义霞\*, 化学学报, 2017, 75(5), 448-452
- Tb@C<sub>82</sub> 异构体的分离及其电化学性质研究 ..... 董薇, 聂梦思, 廉永福\*, 化学学报, 2017, 75(5), 453-456

### 研究论文

- 二价双核铈聚吡咯配合物结构设计和铈-铈多重键的理论研究 ..... 陈方园, 曲宁, 吴群燕, 张红星, 石伟群\*, 潘清江\*, 化学学报, 2017, 75(5), 457-463
- 综合研究 DPE 添加剂对含 5,6-二氟-苯并[1,2,5]噻二唑给-受体共聚物的光伏性能影响 ..... 竹芯, 朱凯, 孙邦锦, 樊健\*, 周祎, 宋波\*, 化学学报, 2017, 75(5), 464-472
- 聚芳撑乙炔微孔骨架材料的合成及其气体吸附 ..... 徐佳伟, 张崇, 王迅昶, 蒋加兴\*, 汪锋\*, 化学学报, 2017, 75(5), 473-478
- Pd/ZSM-5/MCM-41 催化剂加氢脱硫性能研究 ..... 杨晓东\*, 王新苗, 高善彬, 王安杰, 化学学报, 2017, 75(5), 479-484
- 氮掺杂部分石墨化碳/钴铁氧化物复合材料的制备及电化学性能 ..... 李甜甜, 赵继宽\*, 李尧, 全贞兰, 徐洁, 化学学报, 2017, 75(5), 485-493
- 烯酰基-辅酶 A 水合酶催化机理的理论研究 ..... 章瑜, 杨新亚, 于海瀛, 马广才\*, 化学学报, 2017, 75(5), 494-500
- 高倍率球形锂离子电池正极材料  $\text{LiNi}_{0.5}\text{Co}_{0.2}\text{Mn}_{0.3}\text{O}_2$  的制备及其电化学性能研究 ..... 郑卓, 吴振国, 向伟, 郭孝东\*, 化学学报, 2017, 75(5), 501-507
- 二氧化钛光解水过程中乙醇选择性光催化氧化反应研究 ..... 孟超, 王华, 吴煜斌, 付贤智, 员汝胜\*, 化学学报, 2017, 75(5), 508-513

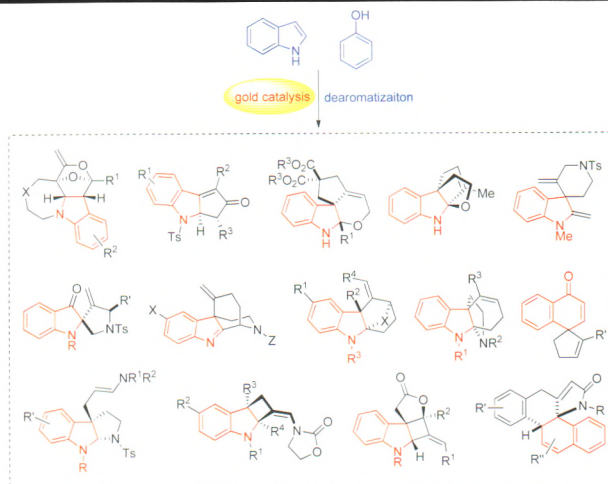
\* 通信联系人.

**On the cover:** Due to its flexibility, tetravalent-anion nature and capability that accommodates bimetallic ions and stabilizes various oxidation states of uranium, a flexible octadentate polypyrrolic Schiff-base macrocycle shows the complexation of two  $U^{IV}$  ions. Compared with the tri- and tetravalent analogous, it is found that the uranium oxidation state is able to tune the energetic matching between the highest-energy occupied orbital of ligand and the adjacent low-energy metal-based orbital, as well as correlates with the metal-ligand electron transfer and the diuranium multiple bond number. [Pan, Qingjiang *et al.* on page 457-463.]



### Perspective

#### Recent Progress on Gold-catalyzed Dearomatization Reactions



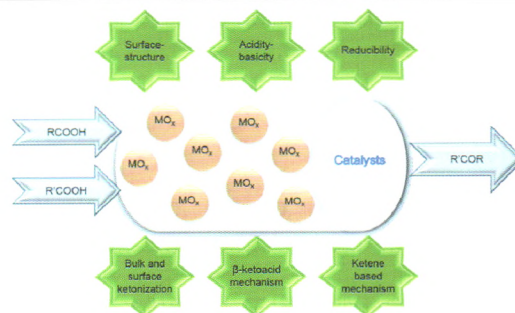
Wu, Wen-Ting; Zhang, Liming\*; You, Shu-Li\*

*Acta Chim. Sinica* **2017**, 75(5), 419-438

Recent examples have demonstrated that gold-catalyzed dearomatization reactions provide a unique and straight way to construct highly functionalized molecules with diverse three-dimensional structures from simple aromatic compounds.

### Review

#### Research Progress in Ketonization of Biomass-derived Carboxylic Acids over Metal Oxides



Ding, Shuang; Ge, Qingfeng; Zhu, Xinli\*

*Acta Chim. Sinica* **2017**, 75(5), 439-447

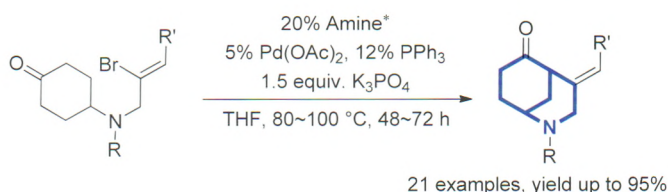
The surface-structure, acidity and basicity, reducibility of metal oxides affect activity of ketonization of carboxylic acids. Various mechanisms have been proposed for ketonization based on different reaction intermediates.

## Communication

Palladium/Amino Acid Co-Catalyzed Intramolecular  $\alpha$ -Vinylolation of Cyclohexanones

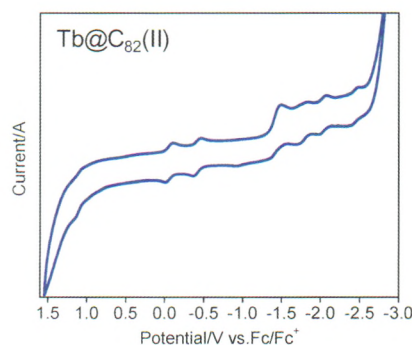
Li, Baole; Liu, Renrong; Liang, Renxiao; Jia, Yixia\*

*Acta Chim. Sinica* **2017**, 75(5), 448-452

Isolation and Electrochemical Property of Tb@C<sub>82</sub> Isomers

Dong, Wei; Nie, Mengsi; Lian, Yongfu\*

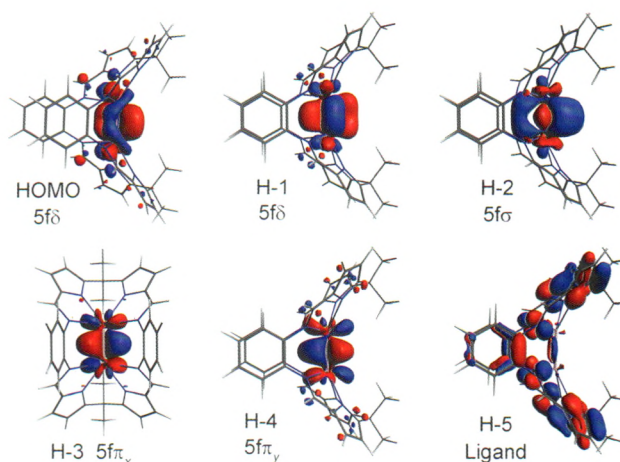
*Acta Chim. Sinica* **2017**, 75(5), 453-456



Two isomers of Tb@C<sub>82</sub> were isolated by three-step high performance liquid chromatography (HPLC) isolation. The carbon cages of isolated Tb@C<sub>82</sub> isomers are estimated to be of C<sub>2v</sub> and C<sub>s</sub> symmetry, respectively, and Tb atom is encapsulated in carbon cage at a valence state of +3. Tb@C<sub>82</sub> (I) exhibits two pairs of reversible oxidative and five pairs of reversible reductive peaks, and Tb@C<sub>82</sub> (II) shows one reversible oxidative and six reversible reductive ones. It is concluded that the symmetry of C<sub>82</sub> cage has little effect on the reduction potentials but great effect on the oxidation potentials of Tb@C<sub>82</sub> isomers.

## Article

## Structures and Uranium-Uranium Multiple Bond of Binuclear Divalent Uranium Complex of Pyrrolic Schiff-base Macrocycle: a Relativistic DFT Probe



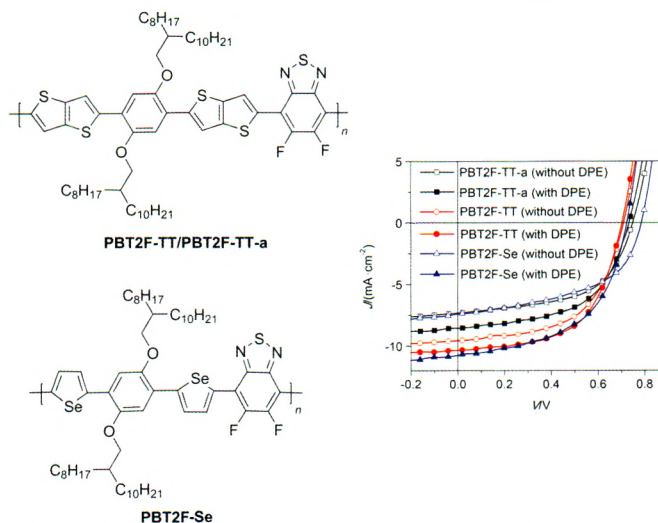
Chen, Fangyuan; Qu, Ning; Wu, Qunyan; Zhang, Hongxing; Shi, Wei-qun\*; Pan, Qingjiang\*

*Acta Chim. Sinica* **2017**, 75(5), 457-463

A relativistic DFT probe has been carried out on the divalent diuranium complex of a single macrocyclic ligand. Its triplet state was found as the ground state. Structural parameters, molecular orbitals and QTAIM analysis all indicate diuranium multiple bonding nature. Comparison with tri- and tetravalent diuranium analogues finds that the uranium oxidation state can tune energetic match between the highest-energy occupied ligand orbital and the adjacent low-energy metal-based orbital, as well as correlates with the electron transfer between metal and ligand and the diuranium multiple bond number.



# Comprehensive Study of the Effect of DPE Additive on Photovoltaic Performance of 5,6-Difluoro-benzo-[1,2,5]-thiadiazole Based Donor-acceptor Copolymers

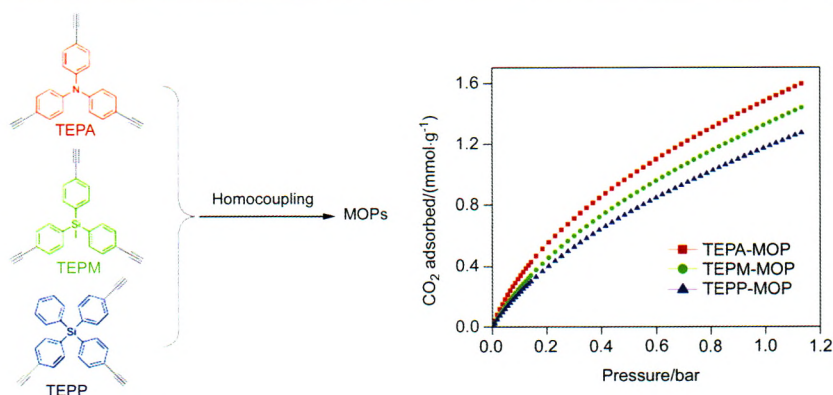


Zhu, Xin; Zhu, Kai; Sun, Bangjin; Fan, Jian\*; Zhou, Yi; Song, Bo\*

*Acta Chim. Sinica* **2017**, 75(5), 464-472

The DPE additive led to the large enhancement in  $J_{SC}$  and PCE of polymer:PC<sub>71</sub>BM blends, which was comprehensively investigated by means of AFM, TEM, alternating current impedance spectrometry, and space-charge-limited current analysis.

# Synthesis and Gas Sorption Properties of Microporous Poly(arylene ethynylene) Frameworks

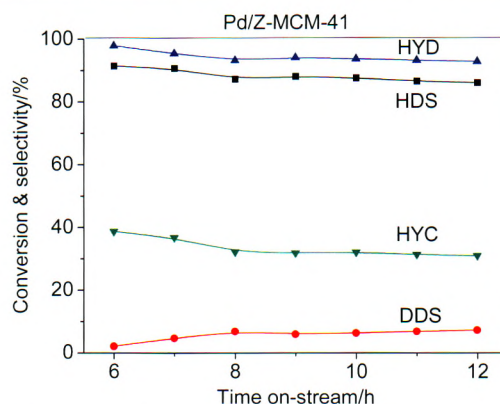


Xu, Jiawei; Zhang, Chong; Wang, Xunchang; Jiang, Jiaxing\*; Wang, Feng\*

*Acta Chim. Sinica* **2017**, 75(5), 473-478

A series of MOPs were synthesized by the oxidative dimerization of terminal alkynes using triethynyl monomers. Among these polymers, TEPA-MOP with the highest BET surface area shows the highest CO<sub>2</sub> uptake capacity of 1.59 mmol g<sup>-1</sup>. As for separation of CO<sub>2</sub>, both TEPA-MOP and TEPP-MOP exhibit relatively high CO<sub>2</sub>-over-N<sub>2</sub> selectivities of 69.9 and 73.2 at 273 K, respectively.

# Hydrodesulfurization Performances of Pd Catalysts Supported on ZSM-5/MCM-41 Composite Zeolite



Yang, Xiaodong\*; Wang, Xinmiao; Gao, Shanbin; Wang, Anjie

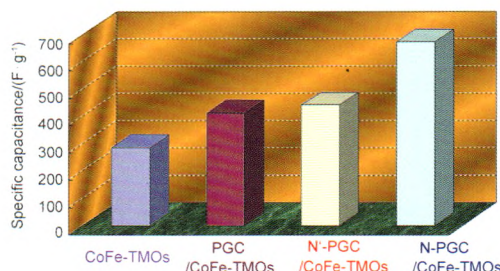
*Acta Chim. Sinica* **2017**, 75(5), 479-484

Pd/Z-MCM-41 exhibited the highest HDS activity and excellent stability. Its enhanced HDS performance may stem from the mesoporous structure and uniform distribution acidity of Z-MCM-41. The acidity of microporous zeolite introduced to mesoporous materials was beneficial to the improvement of HDS activities.

### Synthesis and Electrochemical Properties of Nitrogen-Doped Partially Graphitized Carbon/Cobalt Iron Oxides Composite

Li, Tiantian; Zhao, Jikuan\*; Li, Yao; Quan, Zhenlan; Xu, Jie

*Acta Chim. Sinica* **2017**, 75(5), 485-493

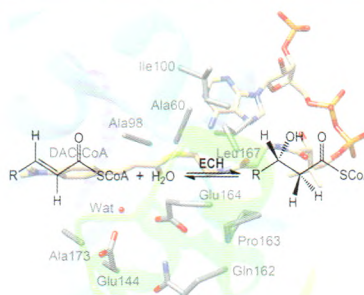


Nitrogen-doped partially graphitized carbon/cobalt iron transition metal oxides nanocomposite (N-PGC/CoFe-TMOs) has been successfully prepared by simple coprecipitation method and calcination treatment, using the biopolymer chitosan as structure directing agent and organic precursor. The N-PGC/CoFe-TMOs nanocomposite is of superior electrochemical property to CoFe-TMOs (pure oxides), PGC/CoFe-TMOs (composite without nitrogen doping), and N'-PGC/CoFe-TMOs (composite with lower carbon content).

### Theoretical Insight into the Catalytic Mechanism of Enoyl-CoA Hydratase

Zhang, Yu; Yang, Xinya; Yu, Haiying; Ma, Guangcai\*

*Acta Chim. Sinica* **2017**, 75(5), 494-500

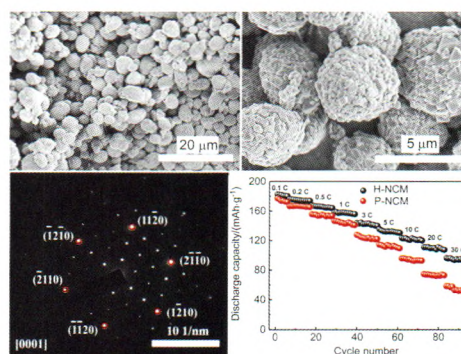


Enoyl-CoA hydratase (ECH) catalyzes the *syn* hydration of  $\alpha,\beta$ -unsaturated thiolester substrates. DFT calculations suggest that hydration reaction proceeds through a stepwise mechanism, involving an enolate intermediate. Glu144 and Glu164, as well as the hydrogen-bonding networks surrounding Glu144 and Glu164 are of great importance for catalysis.

### Preparation and Electrochemical Performance of High Rate Spherical Layered $\text{LiNi}_{0.5}\text{Co}_{0.2}\text{Mn}_{0.3}\text{O}_2$ Cathode Material for Lithium-Ion Batteries

Zheng, Zhuo; Wu, Zhenguo; Xiang, Wei; Guo, Xiaodong\*

*Acta Chim. Sinica* **2017**, 75(5), 501-507

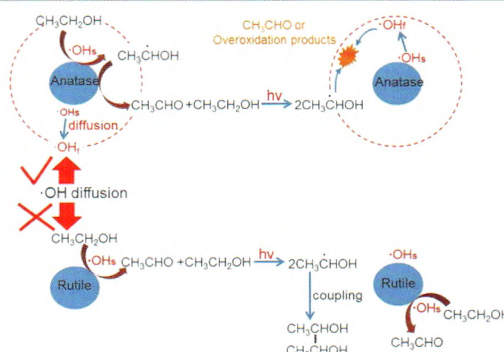


An uniform Ni-rich  $\text{LiNi}_{0.5}\text{Co}_{0.2}\text{Mn}_{0.3}\text{O}_2$  microsphere with an average diameter of *ca.* 5  $\mu\text{m}$  and tap density of 2.1  $\text{g}/\text{cm}^3$  has been prepared by the carbonate co-precipitation method. This as-prepared material has a well-ordered  $\alpha\text{-NaFeO}_2$  structure with stable in-plane  $[\sqrt{3} \times \sqrt{3}]R30^\circ$  ordering in the transition-metal layers, which endows this cathode excellent rate performance and high energy storage capability.

### Study on Selective Photocatalytic Oxidation of Ethanol During $\text{TiO}_2$ Promoted Water-Splitting Process

Meng, Chao; Wang, Hua; Wu, Yubin; Fu, Xianzhi; Yuan, Rusheng\*

*Acta Chim. Sinica* **2017**, 75(5), 508-513



The generation and diffusion of  $\cdot\text{OH}$  from the surface of P25 (80% anatase) to bulk solution is a key step to inhibit the coupling reaction of  $\alpha$ -hydroxyethyl radicals to produce acetaldehyde or overoxidation products. The lack of mobile  $\cdot\text{OH}_f$  on rutile  $\text{TiO}_2$  makes the photochemical reaction between acetaldehyde molecule and ethanol molecule more facile to occur in the heterogeneous system.





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