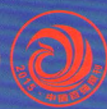


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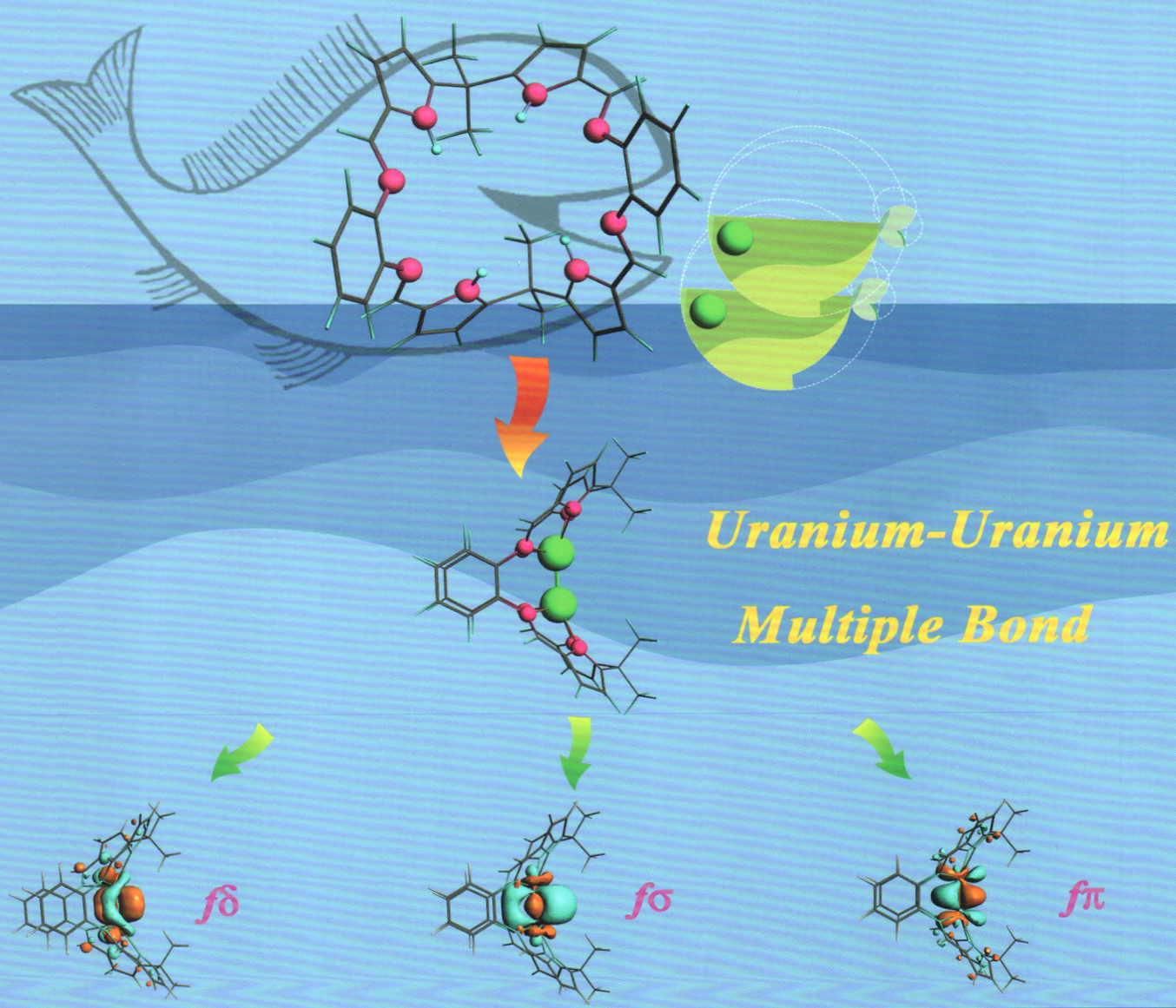


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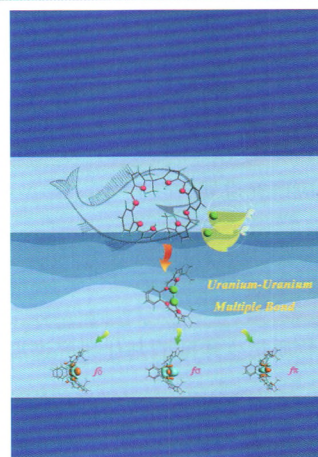
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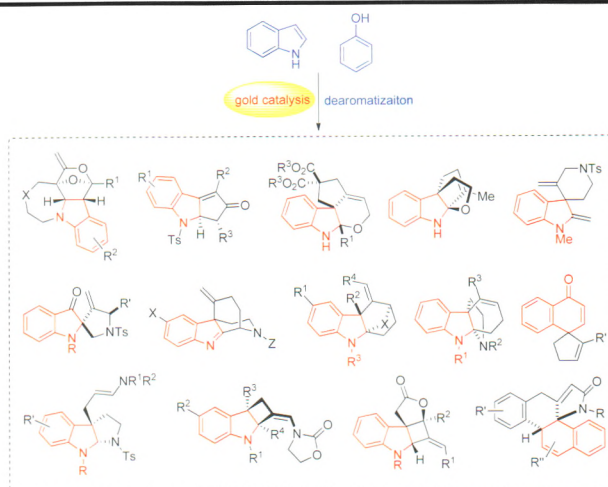
* 通信联系人.

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 polypyrrrolic 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



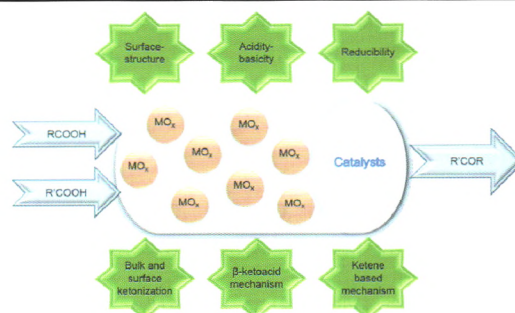
Wu, Wen-Ting; Zhang, Liming*; You, Shu-Li*

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

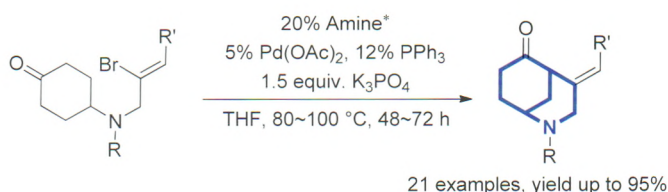
The surface-structure, acidity and basicity, reducibility of metal oxides affect activity of ketonization of carboxylic acids. Various mechanisms have been proposed for ketonization based on different reaction intermediates.

Communication

Palladium/Amino Acid Co-Catalyzed Intramolecular α -Vinylolation of Cyclohexanones

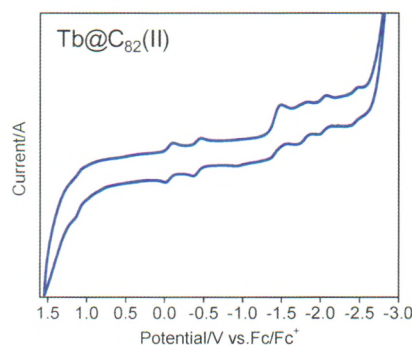
Li, Baole; Liu, Renrong; Liang, Renxiao; Jia, Yixia*

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

Isolation and Electrochemical Property of Tb@C₈₂ Isomers

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

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



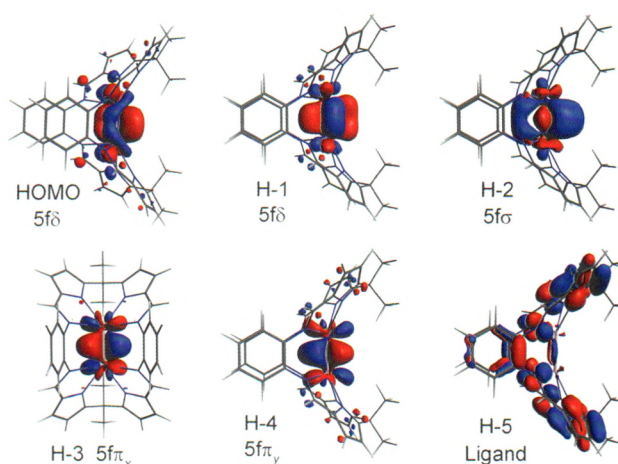
Two isomers of Tb@C₈₂ were isolated by three-step high performance liquid chromatography (HPLC) isolation. The carbon cages of isolated Tb@C₈₂ isomers are estimated to be of C_{2v} and C_s symmetry, respectively, and Tb atom is encapsulated in carbon cage at a valence state of +3. Tb@C₈₂ (I) exhibits two pairs of reversible oxidative and five pairs of reversible reductive peaks, and Tb@C₈₂ (II) shows one reversible oxidative and six reversible reductive ones. It is concluded that the symmetry of C₈₂ cage has little effect on the reduction potentials but great effect on the oxidation potentials of Tb@C₈₂ isomers.

Article

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

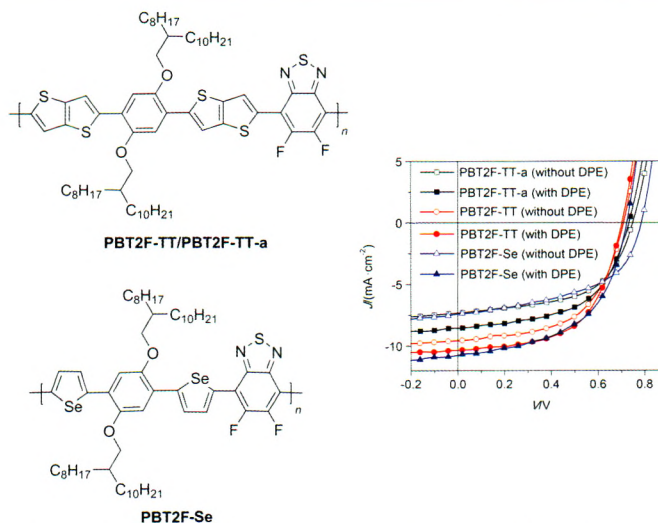
Chen, Fangyuan; Qu, Ning; Wu, Qunyan; Zhang, Hongxing; Shi, Weiqun*; Pan, Qingjiang*

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

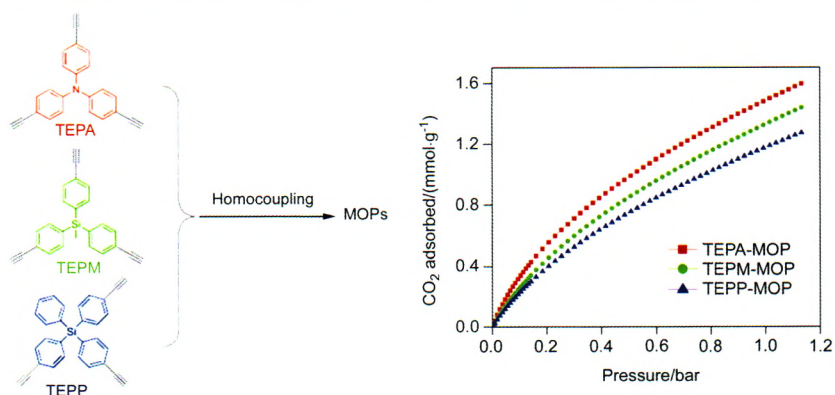


Zhu, Xin; Zhu, Kai; Sun, Bangjin; Fan, Jian*; Zhou, Yi; Song, Bo*

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

The DPE additive led to the large enhancement in J_{SC} and PCE of polymer:PC₇₁BM 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

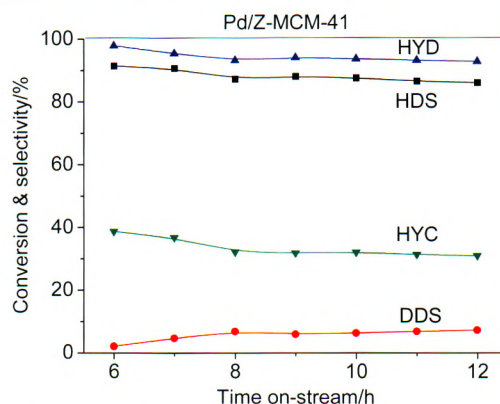


Xu, Jiawei; Zhang, Chong; Wang, Xunchang; Jiang, Jiaying*; Wang, Feng*

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

A series of MOPs were synthesized by the oxidative dimerization of terminal alkynes using triethylaluminum, triethylmagnesium, or triethylpalladium as catalysts. Among these polymers, TEPA-MOP with the highest BET surface area shows the highest CO₂ uptake capacity of 1.59 mmol·g⁻¹. As for separation of CO₂, both TEPA-MOP and TEPP-MOP exhibit relatively high CO₂-over-N₂ 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

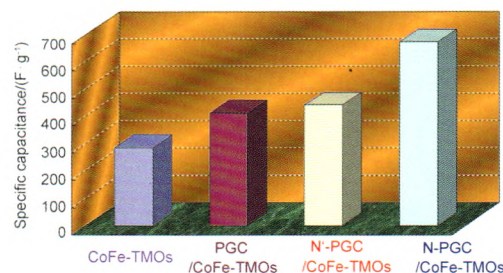
Acta Chim. Sinica **2017**, 75(5), 479-484

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

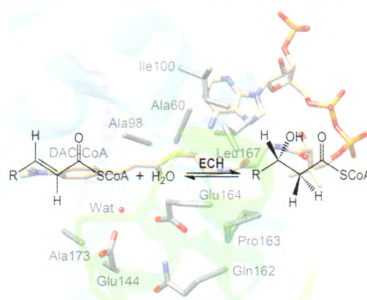


Nitrogen-doped partially graphitized carbon/cobalt iron transition metal oxides nanocomposite (N-PGC/CoFe-TMOs) has been successfully prepared by simple coprecipitation method and calcination treatment, using the biopolymer chitosan as structure directing agent and organic precursor. The N-PGC/CoFe-TMOs 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

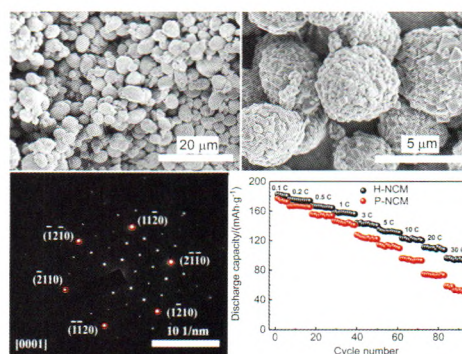


Enoyl-CoA hydratase (ECH) catalyzes the *syn* hydration of α,β -unsaturated thioester substrates. DFT calculations suggest that hydration reaction proceeds through a stepwise mechanism, involving an enolate intermediate. Glu144 and Glu164, as well as the hydrogen-bonding networks surrounding Glu144 and 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

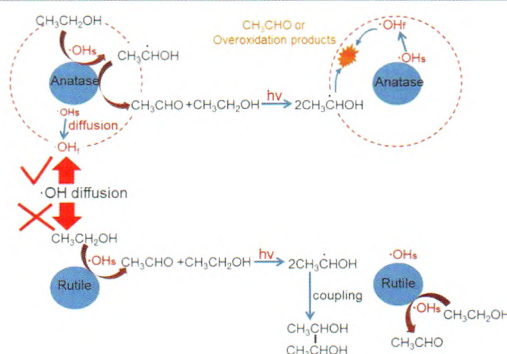


An uniform Ni-rich $\text{LiNi}_{0.5}\text{Co}_{0.2}\text{Mn}_{0.3}\text{O}_2$ microsphere with an average diameter of *ca.* 5 μm and tap density of 2.1 g/cm^3 has been prepared by the carbonate co-precipitation method. This as-prepared material has a well-ordered $\alpha\text{-NaFeO}_2$ structure with 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 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 α -hydroxyethyl radicals to produce acetaldehyde or overoxidation products. The lack of mobile $\cdot\text{OH}_f$ on rutile TiO_2 makes the photochemical reaction between acetaldehyde molecule and ethanol molecule more facile to occur in the heterogeneous system.



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