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IN THIS ISSUE

ISSN 1477-9226 CODEN DTARAF 53(5) 1881–2396 (2024)



Cover

See Kunio Awaga et al.,
pp. 1961–1965.

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Inside cover

See Matthias Tamm et al.,
pp. 1942–1946.

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1942.

We would like to thank Dr.
Thomas Bannenberg for pro-
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EDITORIAL

1897

Spotlight collection on inorganic molecular electronics

Cláudio N. Verani* and Paul J. Low*

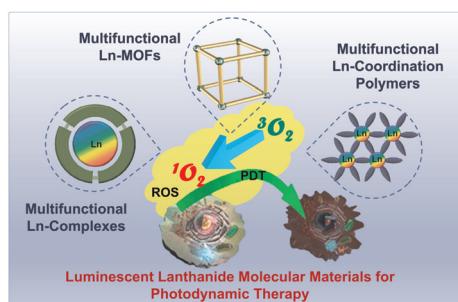


PERSPECTIVES

1898

Luminescent lanthanide-based molecular materials: applications in photodynamic therapy

M. L. P. Reddy* and K. S. Bejoymohandas



Environmental Science: Atmospheres



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Fundamental questions
Elemental answers



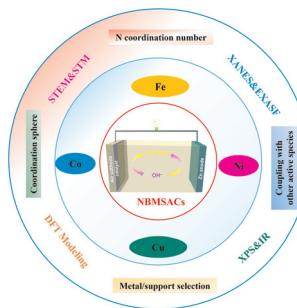
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PERSPECTIVES

1915

Non-noble metal single-atoms for oxygen electrocatalysis in rechargeable zinc–air batteries: recent developments and future perspectives

Le Li,* Jixing Xu, Qianyi Zhu, Xiangjun Meng, Hongliang Xu and Meijun Han

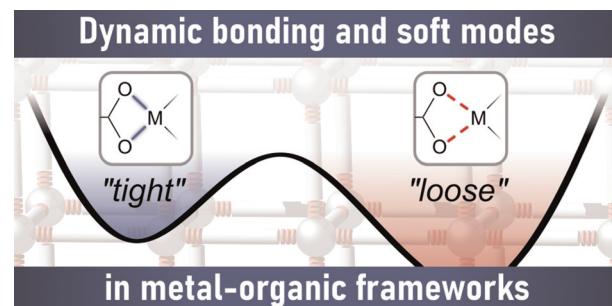


FRONTIER

1935

Dynamic metal-linker bonds in metal–organic frameworks

Erik Svensson Grape, Audrey M. Davenport and Carl K. Brozek*

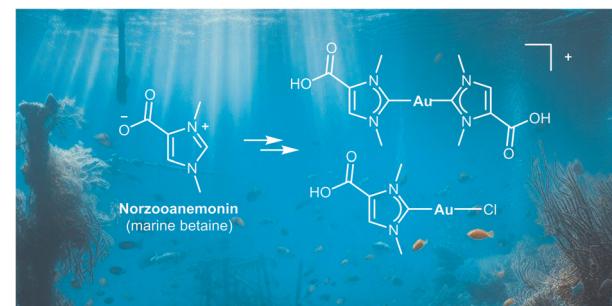


COMMUNICATIONS

1942

Synthesis of N-heterocyclic carbene gold(I) complexes from the marine betaine 1,3-dimethylimidazolium-4-carboxylate

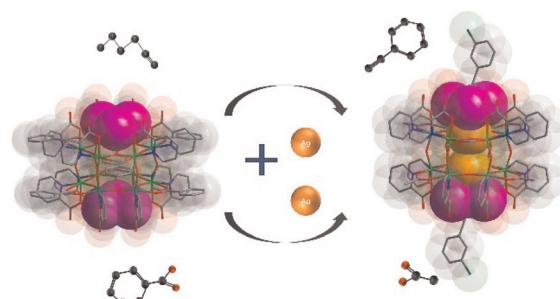
Seyedeh Mahbobe Mahdavi, Dirk Bockfeld, Rolf Büsing, Bianka Karge, Thomas Bannenberg, René Frank, Mark Brönstrup, Ingo Ott and Matthias Tamm*



1947

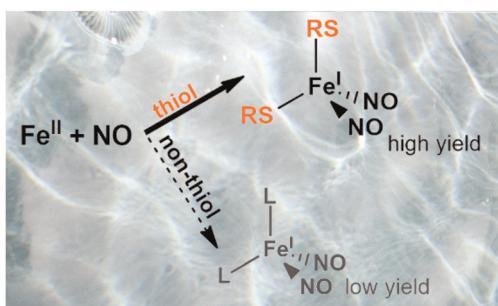
Structure and optical limiting effects of heterometallic $\text{Ag}_6@\text{Ti}_{12}$ and $\text{Ag}_8@\text{Ti}_{12}$ oxo clusters regulated by alkynyl ligands

Li-Jun Rong, Yu-Ting Ye, Xin Lin, Xiaohui Sun, Shumei Chen,* Jian Zhang and Lei Zhang*



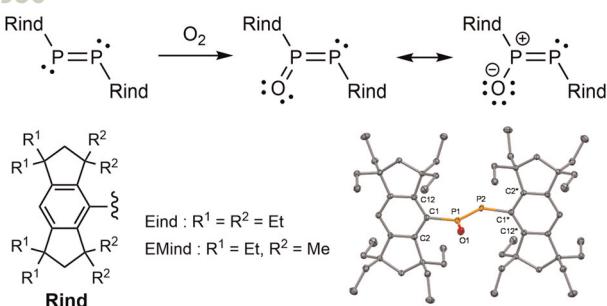
COMMUNICATIONS

1951

**Insight into the relevance of dinitrosyl iron complex (DNIC) formation in the absence of thiols in aqueous media**

Nathália Miranda Medeiros, Felipe Alves Garcia and Daniela Ramos Truzzi*

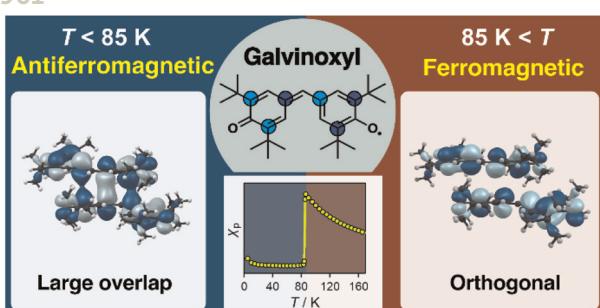
1956

**Selective monooxygenation of diphosphenes with molecular oxygen**

Yuria Kawase, Shota Tsujimoto, Tomohiro Obayashi, Satoshi Kimura, Kanta Ito, Shotaro Ikoma, Kei Ota, Daisuke Hashizume and Tsukasa Matsuo*

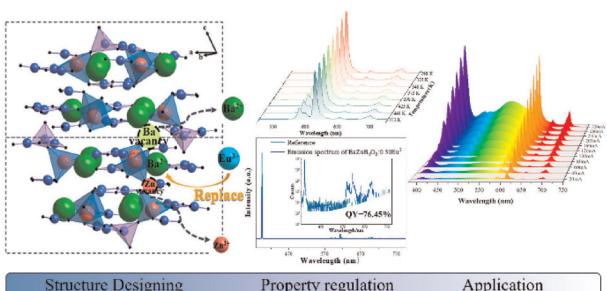
PAPERS

1961

**X-ray crystallographic analysis of the antiferromagnetic low-temperature phase of galvinoxyl: investigating magnetic duality in organic radicals**

Rie Suizu, Yoshiaki Shuku, Vincent Robert, Pablo Roseiro, Nadia Ben Amor, Zain Khawar, Neil Robertson and Kunio Awaga*

1966

**Cation vacancy-boosted $\text{BaZnB}_4\text{O}_{8:x}\text{Eu}^{3+}$ phosphors with high quantum yield and thermal stability for pc-WLEDs**

Naijia Liu, Nianmin Chen, Yunjian Wang,* Juanjuan Kong and Zhe Wang*

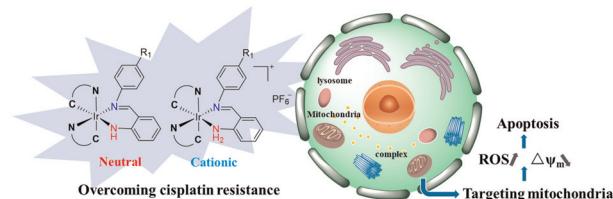


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1977

Mitochondria-targeted neutral and cationic iridium(III) anticancer complexes chelating simple hybrid $sp^2\text{-N}/sp^3\text{-N}$ donor ligands

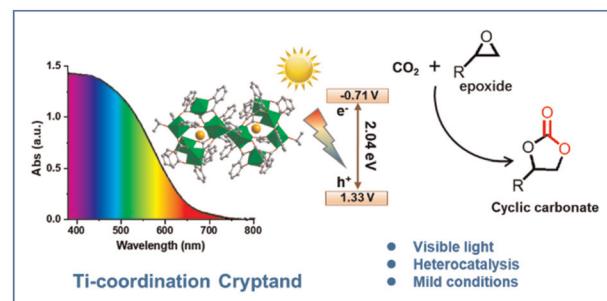
Pengwei Li, Lihua Guo,* Jiaxing Li, Zhihao Yang, Hanxiu Fu, Kangning Lai, Heqian Dong, Chunyan Fan and Zhe Liu*



1989

A cryptand-like Ti-coordination compound with visible-light photocatalytic activity in CO_2 storage

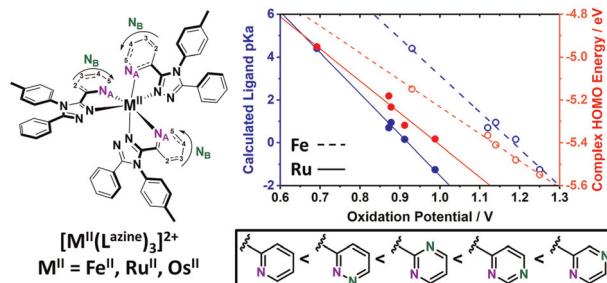
Yanshu Liu, Guanyun Zhang,* Dexin Wang, Guanjie Chen, Fangfang Gao, Chen-Ho Tung and Yifeng Wang*



1999

Predictable electronic tuning of Fe^{II} and Ru^{II} complexes *via* choice of azine: correlation of ligand pK_a with $E_{pa}(\text{M}^{III/II})$ of complex

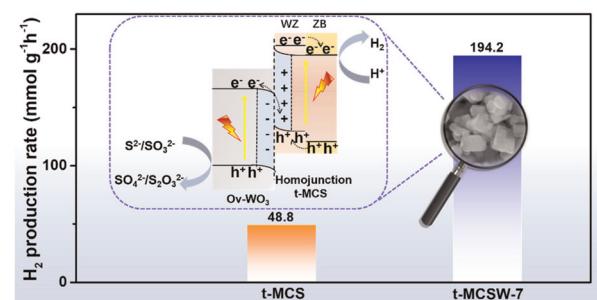
Matthew G. Robb, Luca Bondi, Santiago Rodríguez-Jiménez, Anna L. Garden, Paul Jerabek* and Sally Brooker*



2008

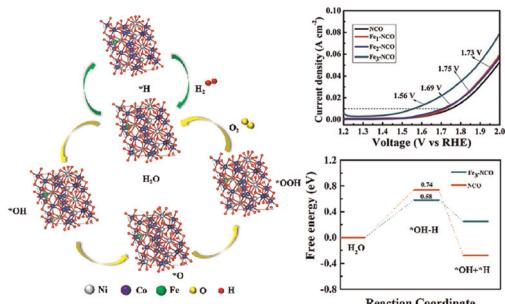
Synergistic optimization of triple phase junctions and oxygen vacancies over $\text{Mn}_x\text{Cd}_{1-x}\text{S}/\text{Ov-WO}_3$ for boosting photocatalytic hydrogen evolution

Haitao Zhao,* Hongjie Zhu, Min Wang, Heyuan Liu and Xiyou Li*



PAPERS

2018

**Iron-doping-induced formation of Ni–Co–O nanotubes as efficient bifunctional electrodes**

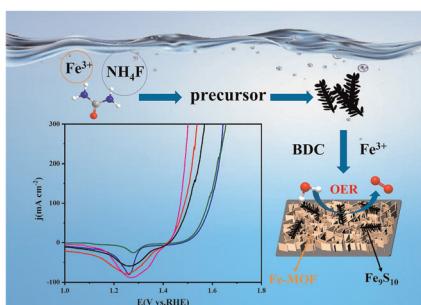
Zhaohui Liu,* Xinjiang Zhang, Xiaona Mi, Zirun Yang and Haihua Huang*

2029

**Synthesis, crystal and electronic structures, linear and nonlinear optical properties, and photocurrent response of oxyhalides CeHaVIO₄ (Ha = Cl, Br; VI = Mo, W)**

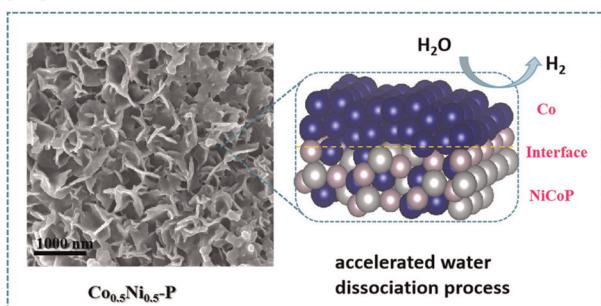
Zixian Jiao, Jasmine Quah, Tajamul Hussain Syed, Wei Wei, Bingbing Zhang, Fei Wang* and Jian Wang*

2039

**Ultrathin Fe-MOFs modified by Fe₉S₁₀ for highly efficient oxygen evolution reaction**

Wenjing Shang, Binghao Wang, Xin Deng, Yiqin Tian, Yongbing Lou and Jinxi Chen*

2048

**Heterogeneous Co–Ni phosphide with active sites for water dissociation and efficient hydrogen evolution reaction**

Nan Jiang,* Jiayou Li, Bing Wang, Yuhan Zhang, Weijun Gao and Bolong Jiang*

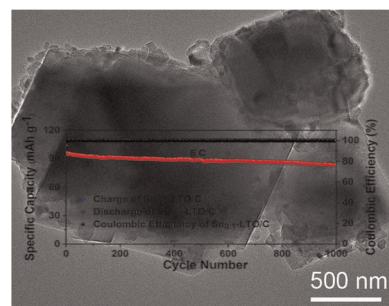


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2055

Sn_{0.1}-Li₄Ti₅O₁₂/C as a promising cathode material with a large capacity and high rate performance for Mg–Li hybrid batteries

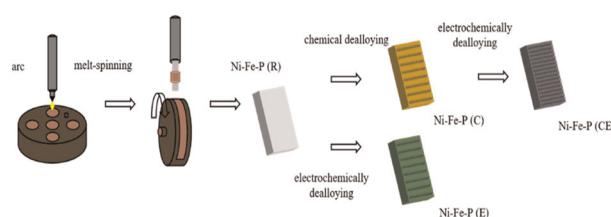
Wei Lin, Xingwei Zuo, Chao Ma, Peng Xia, Haowei Bian, Guobing Liang, Jianbing Hu, Zhongcheng Song, Wutao Mao* and Keyan Bao*



2065

Modulating nickel-iron active species via dealloying to boost the oxygen evolution reaction

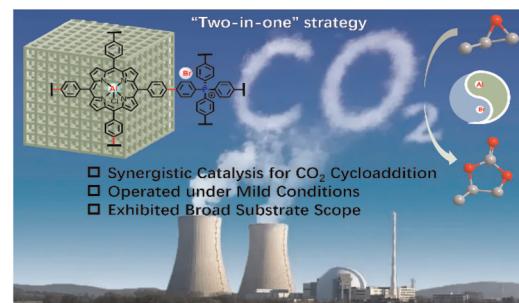
Zhuqing Wan, Xiaolong Guo,* Junying Jiang, Yuci Xin, Benzhen Tang, Hong Zhang, Yong Wu,* Lei Xia and Peng Yu*



2073

Two in one: aluminum porphyrin-based porous organic polymers containing symmetrical quaternary phosphonium salts for catalytic conversion of CO₂ into cyclic carbonates

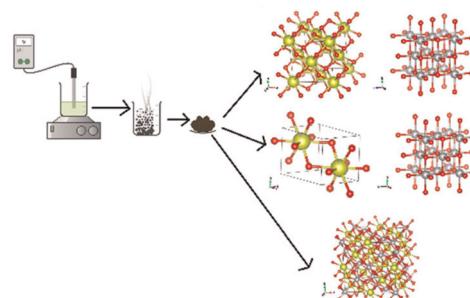
Kechi Chen, Yuanxiang Wu, Zixuan Zhang, Yiying Yang and Rongchang Luo*



2082

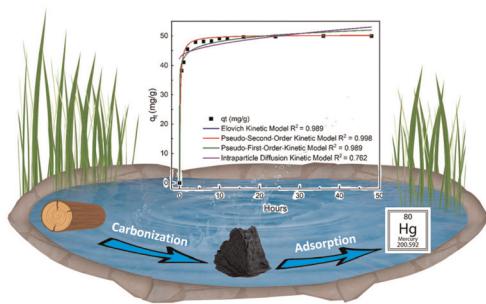
Resolving a structural issue in cerium-nickel-based oxide: a single compound or a two-phase system?

Jelena Kojčinović, Dalibor Tatar, Stjepan Šarić, Cora Bartus Pravda, Andraž Mavrič, Iztok Arčon, Zvonko Jagličić, Maximilian Mellin, Marcus Einert, Angela Altomare, Rocco Caliandro, Ákos Kukovecz, Jan Philipp Hofmann and Igor Djerdj*



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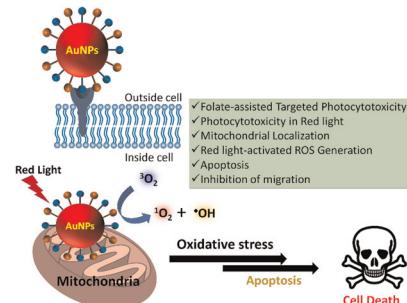
2098



Sulfur functionalized biocarbon sorbents for low-concentration mercury isolation

Douglas Austin, Kousar Jahan, Xu Feng, Jared Carney, Dale K. Hensley, Jihua Chen, Brianna E. Altidor, Zhiyong Guo,* Elizabeth Michaelis, Mariana K. Kebaso and Yanfeng Yue*

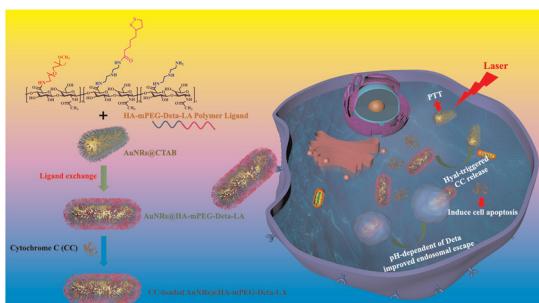
2108



Folate-assisted targeted photocytotoxicity of red-light-activatable iron(III) complex co-functionalized gold nanoconjugates (Fe@FA-AuNPs) against HeLa and triple-negative MDA-MB-231 cancer cells

Maynak Pal, Aarti Upadhyay, Neha Masarkar, Arpan Bera, Sukhes Mukherjee and Mithun Roy*

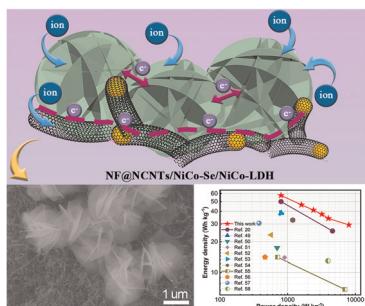
2120



A tumor-targeted and enzyme-responsive gold nanorod-based nanoplateform with facilitated endo–lysosomal escape for synergistic photothermal therapy and protein therapy

Bo Wang, Xin Jun Xu, Yan Fu, Bo Ren,* Xiao Dong Yang* and Hong Yu Yang*

2131



NiCo-compounds inside and outside N-doped carbon nanotubes to construct a double-enhanced hierarchical structure for high energy density supercapacitors

Lansen Bi, Qingbin Tian, Lei Geng, Yang Zhou, Benyu Zheng, Jiang-Shan Gao* and Yan He*

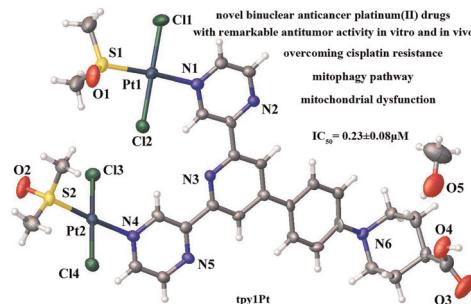


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2143

Synthesis and anticancer mechanisms of four novel platinum(II) 4'-substituted-2,2':6',2''-terpyridine complexes

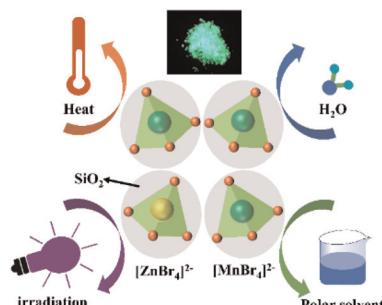
Chun-Jie Liang, Run-Chun Wu, Xiao-Qiong Huang, Qi-Pin Qin,* Hong Liang and Ming-Xiong Tan*



2153

Highly efficient and stable $\text{Cs}_3\text{Mn}_{0.93}\text{Zn}_{0.07}\text{Br}_5@\text{SiO}_2$ for wide color gamut backlight displays

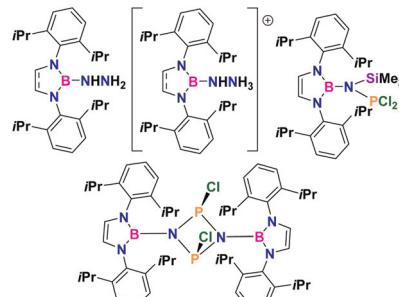
Chun Sun,* Zhihui Deng, Xiaohui Liu, Fuhao Zhang, Kai Lian, Yiwei Zhao, Hu Zhang, Jiachen Han and Mingming Luo*



2159

Boron diamide derivatives containing N–N and N–P molecular fragments

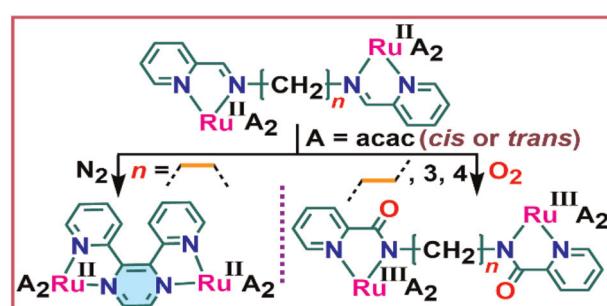
Christopher J. Major, Shi-Ming Chen and Douglas W. Stephan*



2167

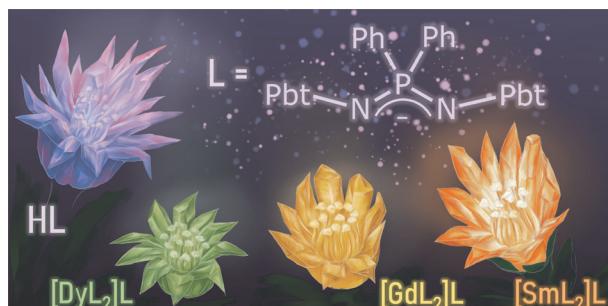
Metal–ligand synergy driven functionalisation of alkylene linked bis(aldimine) on a diruthenium(II) platform. Cyclisation versus oxygenation

Mitrali Biswas, Sanchaita Dey, Suman Dhara, Sanjib Panda and Goutam Kumar Lahiri*



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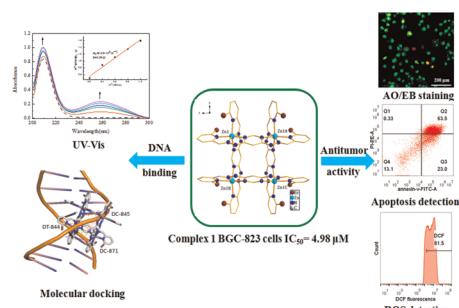
2181



Lanthanide complexes with a new luminescent iminophosphonamide ligand bearing phenylbenzothiazole substituents

Dmitry K. Sinitsa, Ekaterina K. Pylova, Olga A. Mironova,* Denis A. Bashirov, Alexey A. Ryadun, Taisiya S. Sukhikh and Sergey N. Konchenko*

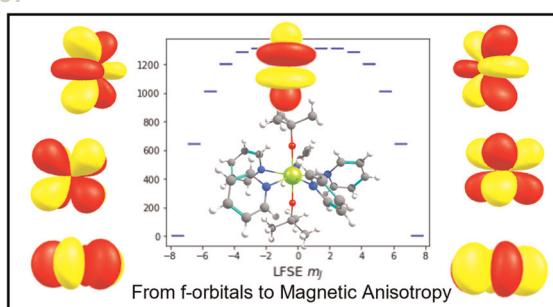
2193



Novel tetranuclear grid-like Zn(II) complexes derived from dihydrazone pyrimidine derivatives as antitumor agents

Juan Yuan,* Hai-Rong Lan, Ai-Ping Xing, Dai Zeng, Ya-Ting Hao, Jun-Ying Song,* Jia-Xing Lu, Bin Zhang, Jing Wang and Zhen-Qiang Zhang*

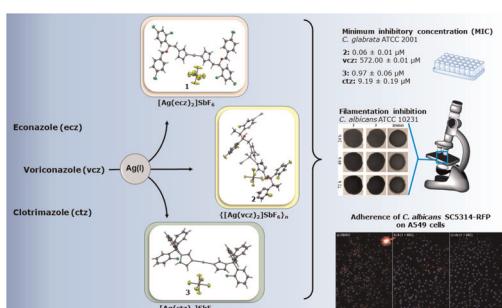
2207



Understanding Single-Molecule Magnet properties of lanthanide complexes from 4f orbital splitting

Yolimar Gil and Daniel Aravena*

2218



Silver(I) complexes containing antifungal azoles: significant improvement of the anti-*Candida* potential of the azole drug after its coordination to the silver(I) ion

Mia Stanković, Jakob Kljun, Nevena Lj. Stevanović, Jelena Lazic, Sanja Skaro Bogojević, Sandra Vojnović, Matija Zlatar, Jasmina Nikodinovic-Runic, Iztok Turel,* Miloš I. Djuran* and Biljana Đ. Glišić*

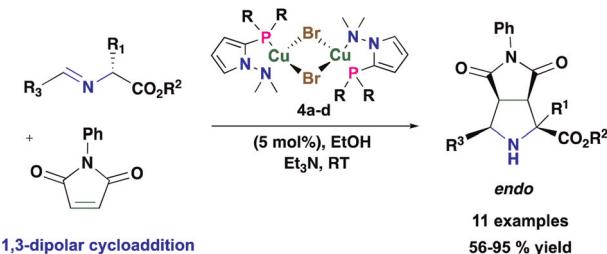


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2231

Well-defined Cu(I) complexes based on [N,P]-pyrrole ligands catalyzed a highly endoselective 1,3-dipolar cycloaddition

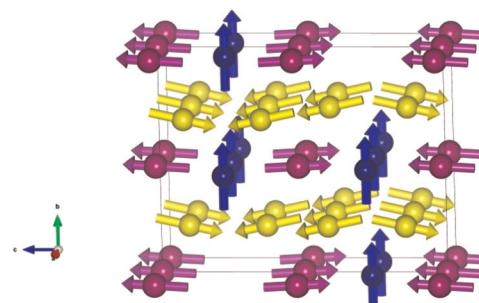
Miguel A. Alvarado-Castillo, Salvador Cortés-Mendoza, José E. Barquera-Lozada, Francisco Delgado,* Rubén A. Toscano, M. Carmen Ortega-Alfaro and José G. López-Cortés*



2242

Orthogonal magnetic structures of Fe_4O_5 : representation analysis and DFT calculations

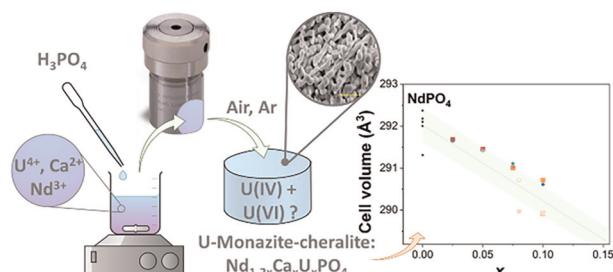
Vyacheslav S. Zhandun,* Natalia V. Kazak, Ilya Kupenko, Denis M. Vasiukov, Xiang Li, Elizabeth Blackburn and Sergei G. Ovchinnikov



2252

Incorporation of U(IV) in monazite–cheralite ceramics under oxidizing and inert atmospheres

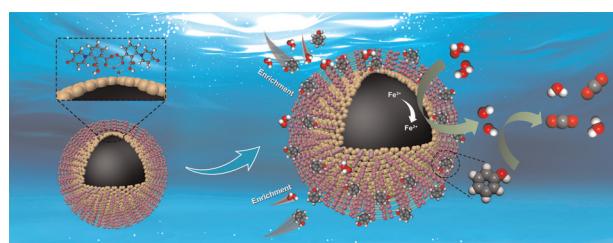
Alison El Monjid, Stéphanie Szenknect,* Adel Mesbah, Myrtille O. J. Y. Hunault, Denis Menut, Nicolas Clavier and Nicolas Dacheux



2265

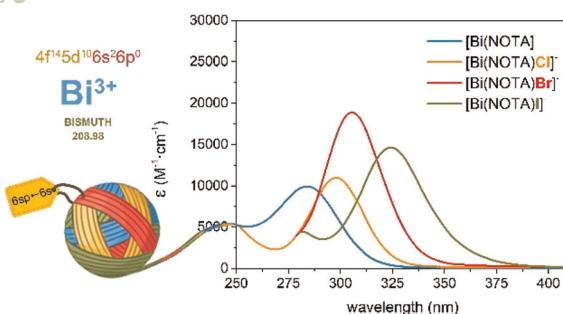
Electron-deficient $\text{Fe}_3\text{O}_4@\text{AC}-\text{NH}_2@\text{Cu-MOF}$ nanoparticles for enhanced degradation of electron-rich benzene derivatives via synergistic adsorption and catalytic oxidation

Qingpeng Cao,* Mengjia Huang, Libin Qian, Jin Wang, Di Wang* and Xubin Zheng*



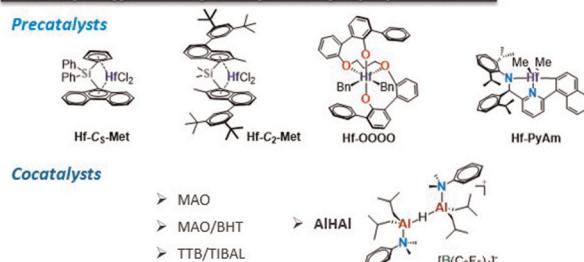
PAPERS

2275

**Unravelling the 6sp ← 6s absorption spectra of Bi(III) complexes**

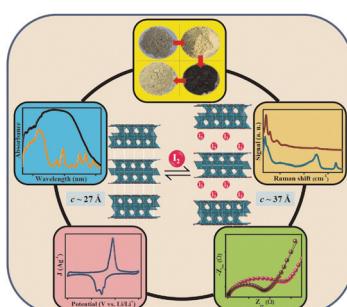
Charlene Harriswangler, Fátima Lucio-Martínez, Aurora Rodríguez-Rodríguez, David Esteban-Gómez and Carlos Platas-Iglesias*

2286

Cocatalyst effects in Hf-catalyzed olefin polymerization**Cocatalyst effects in Hf-catalysed olefin polymerization: taking well-defined Al-alkyl borate salts into account**

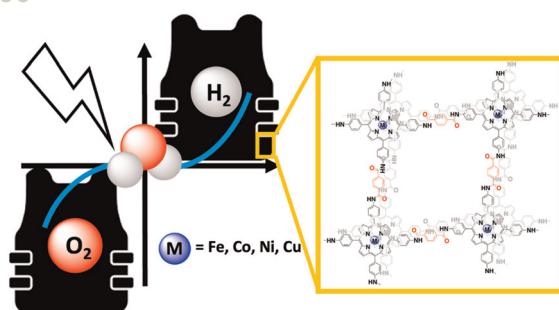
Gaia Urciuoli, Francesco Zaccaria,* Cristiano Zuccaccia, * Roberta Cipullo,* Peter H. M. Budzelaar, Antonio Vittoria, Christian Ehm, Alceo Macchioni and Vincenzo Busico

2294

**Quasi-2D $\text{Bi}_{0.775}\text{Ln}_{0.225}\text{O}_{1.5}$ ($\text{Ln} = \text{La, Pr, Nd, Sm, Eu}$): reversible iodine intercalation and their evaluation as the anode in the lithium-ion battery system**

Priyanka Yadav, Shivangi Rao, O. V. Sreejith, Ramaswamy Murugan and Rajamani Nagarajan*

2306

**Bifunctional porphyrin-based metal-organic polymers for electrochemical water splitting**

Neidy Ocuane, Yulu Ge, Christian Sandoval-Pauker and Dino Villagrán*

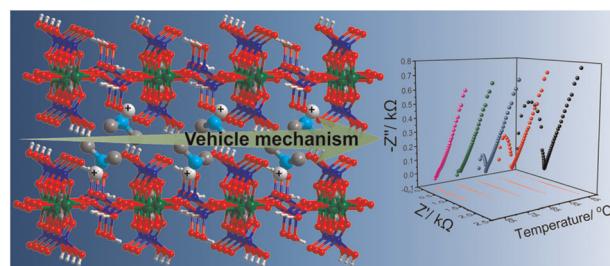


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2318

New group IIIA metal phosphate–oxalates containing dimethylammonium cations with proton conductivity

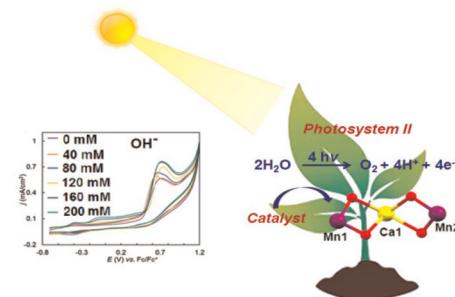
Tian-Yu Pan, Wei-Yang Wen, Wen Ma,*
Shou-Tian Zheng, Mei-Ling Feng* and Xiao-Ying Huang



2324

Chemistry of a series of heterobimetallic complexes $Mn^{III}_2(Ca^{II}/Sr^{II})X_2$ ($X = Cl^-$, Br^-)

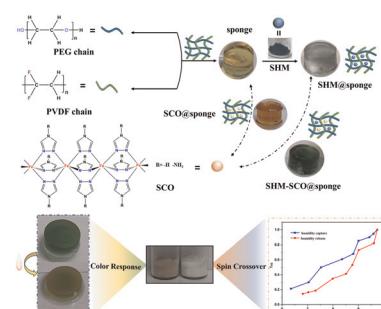
Priyabrata Bhattacharya, Riya Bag, Ray J. Butcher,
Snehanjali Behera, Biswajit Mondal* and
Sanchita Goswami*



2333

Construction and screening of spin-crossover-sponge materials based on iron(II)-triazole coordination polymers

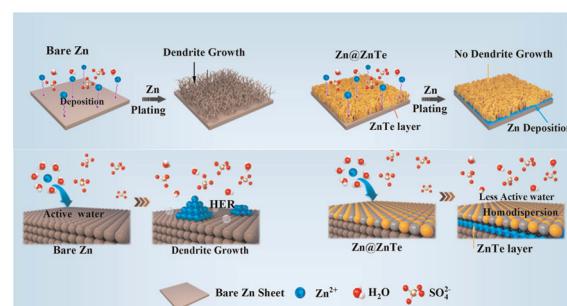
Feng-Lian Zeng, Xue-Ting Jin, Jie Zhao, Shu-Xin Zhang,
Cheng Xue and Yang-Hui Luo*



2341

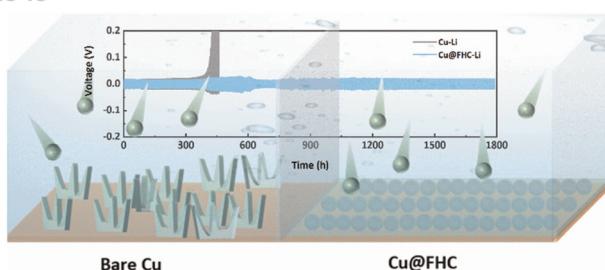
Surface modulation of zinc anodes by foveolate ZnTe nanoarrays for dendrite-free zinc ion batteries

Yi He, Cong Wang,* Yaping Gan, Lingzhi Kang, Lei Xie,
Yuhao He, Zhihui Wu, Guotong Tong, Heng Zhang* and
Qiang Hu*



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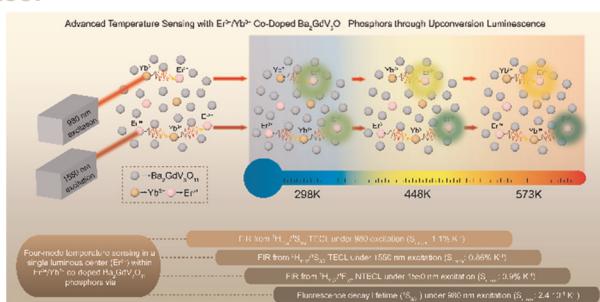
2349



Synergistic regulation of Li deposition on F-doped hollow carbon spheres toward dendrite-free lithium metal anodes

Jianzong Man,* Jinpeng Yin, Wenlong Liu, Xiaodong Sun, Dong Wang, Yongfu Cui and Juncai Sun*

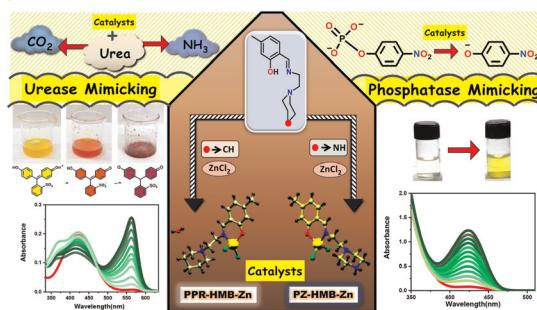
2357



Advanced temperature sensing with Er³⁺/Yb³⁺ co-doped Ba₂GdV₃O₁₁ phosphors through upconversion luminescence

Ikhlas Kachou, Kamel Saidi, Utku Ekim, Mohamed Dammak,* Miray Çelikbilek Ersundu and Ali Erçin Ersundu*

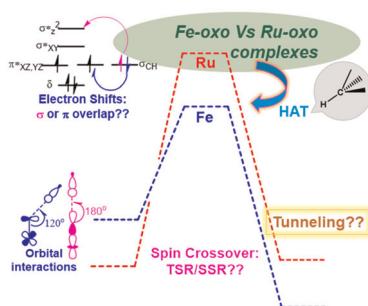
2373



Comparative analysis of Zn(II)-complexes as model metalloenzymes for mimicking Jack bean urease

Rinku Ghanta, Tania Chowdhury,* Avik Ghosh, Avijit K. Das and Tanmay Chattopadhyay*

2386



High-valent nonheme Fe(IV)O/Ru(IV)O complexes catalyze C–H activation reactivity and hydrogen tunneling: a comparative DFT investigation

Akanksha Katoch and Debasish Mandal*

