

# Chemical Science

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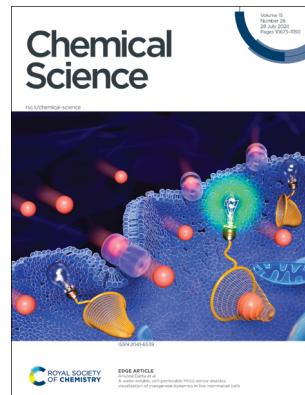
## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(28) 10673–11150 (2024)



### Cover

See Gustavo Fernández et al., pp. 10745–10752. Image reproduced by permission of Gustavo Fernández from *Chem. Sci.*, 2024, 15, 10745.



### Inside cover

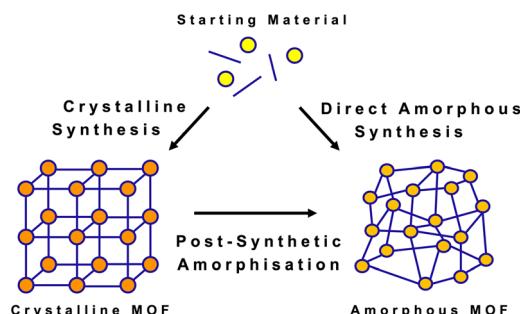
See Ankona Datta et al., pp. 10753–10769. Image reproduced by permission of Ankona Datta from *Chem. Sci.*, 2024, 15, 10753.

## PERSPECTIVE

10689

### Synthetic and analytical considerations for the preparation of amorphous metal–organic frameworks

Emily V. Shaw, Ashleigh M. Chester, Georgina P. Robertson, Celia Castillo-Blas and Thomas D. Bennett\*

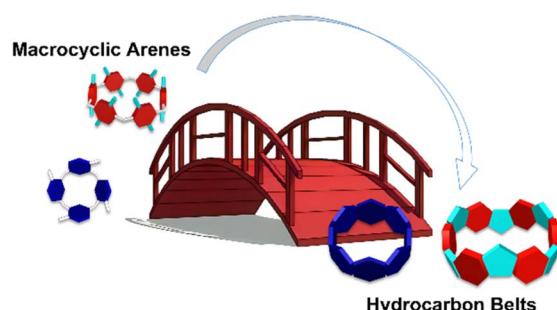


## REVIEWS

10713

### Construction of hydrocarbon belts based on macrocyclic arenes

Guangtan Fan, Zhi Zhang, Guangguo Wang, Li Shao, Bin Hua\* and Feihe Huang\*



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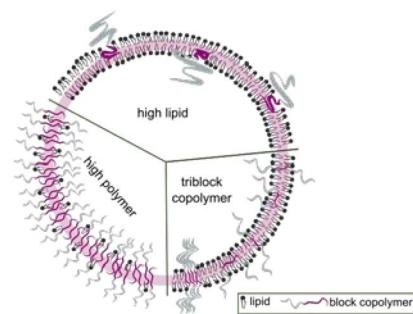
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## REVIEWS

10724

**Advances in block copolymer-phospholipid hybrid vesicles: from physical–chemical properties to applications**

Edit Brodszki\* and Brigitte Städler



## EDGE ARTICLES

10745

**Pathway-dependent supramolecular polymerization by planarity breaking**

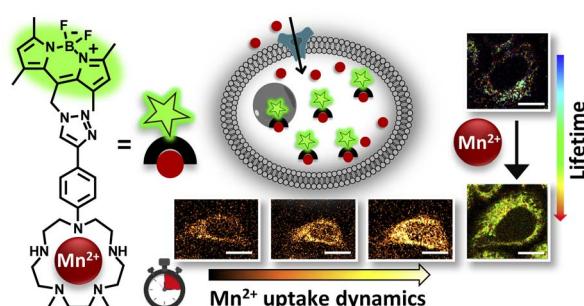
Rasitha Manha Veedu, Zulema Fernández, Nils Bäumer, Antonia Albers and Gustavo Fernández\*



10753

**A water-soluble, cell-permeable Mn(II) sensor enables visualization of manganese dynamics in live mammalian cells**

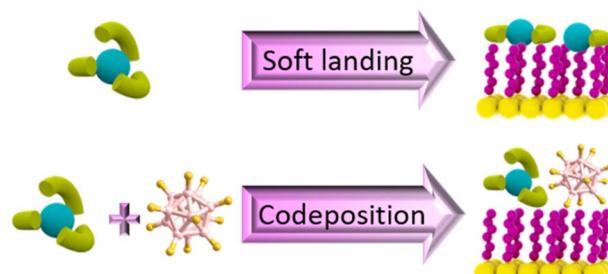
Smitaroop Kahali, Sujit Kumar Das, Ravinder Kumar, Kunika Gupta, Rajasree Kundu, Baivabi Bhattacharya, Arnab Nath, Ravindra Venkatramani and Ankona Datta\*



10770

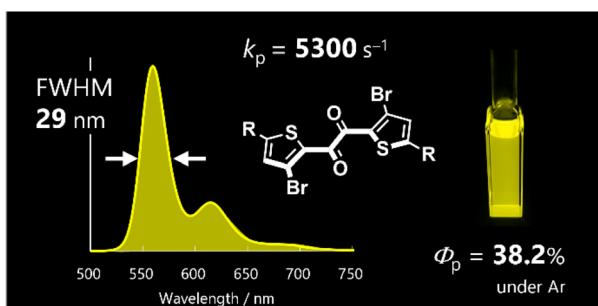
**Spontaneous ligand loss by soft landed  $[\text{Ni}(\text{bpy})_3]^{2+}$  ions on perfluorinated self-assembled monolayer surfaces**

Hugo Y. Samayoa-Oviedo, Harald Knorke, Jonas Warneke\* and Julia Laskin\*



## EDGE ARTICLES

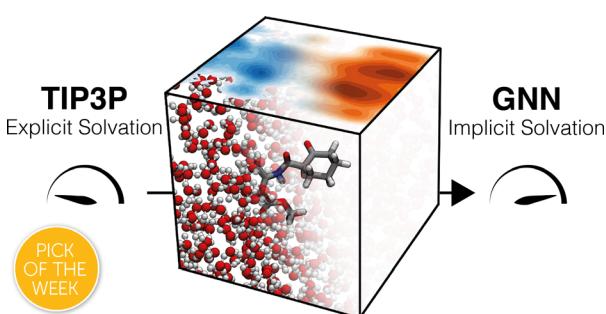
10784



**Fast, efficient, narrowband room-temperature phosphorescence from metal-free 1,2-diketones: rational design and the mechanism**

Yosuke Tani,\* Kiyoshi Miyata,\* Erika Ou, Yuya Oshima, Mao Komura, Morihisa Terasaki, Shuji Kimura, Takumi Ehara, Koki Kubo, Ken Onda and Takuji Ogawa

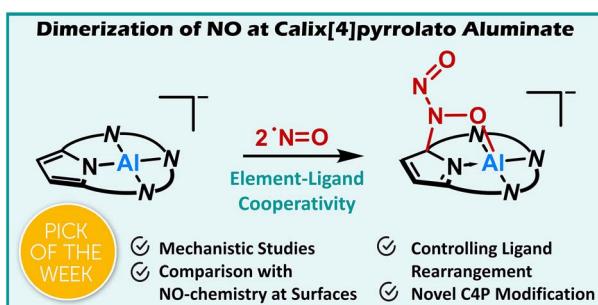
10794



**A general graph neural network based implicit solvation model for organic molecules in water**

Paul Katzberger and Sereina Riniker\*

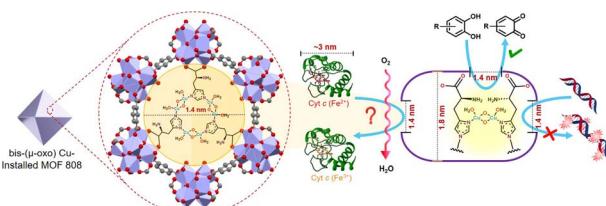
10803



**Nitrogen monoxide and calix[4]pyrrolato aluminate: structural constraint enabled NO dimerization**

Senta J. Kohl, Lukas M. Sigmund, Manuel Schmitt and Lutz Greb\*

10810



**Approach of a small protein to the biomimetic bis-( $\mu$ -oxo) dicopper active-site installed in MOF-808 pores with restricted access perturbs substrate selectivity of oxidase nanozyme**

Rasmi V. Morajkar, Adarsh P. Fatrekar and Amit A. Vernekar\*

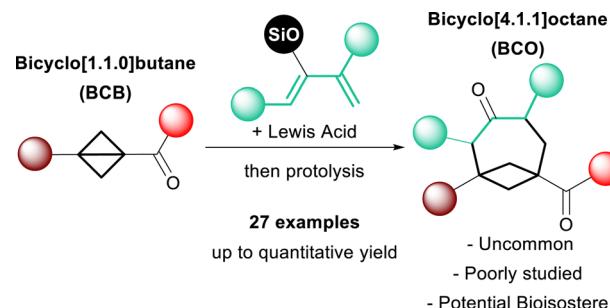


## EDGE ARTICLES

10823

**Lewis acid catalyzed [4+2] annulation of bicyclobutanes with dienol ethers for the synthesis of bicyclo[4.1.1]octanes**

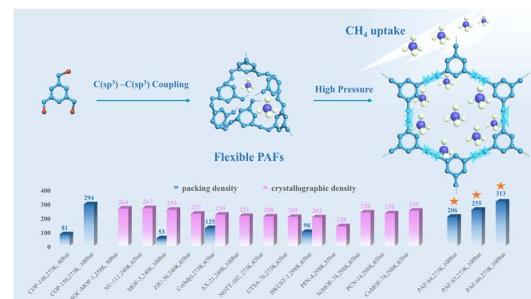
Stefano Nicolai\* and Jérôme Waser\*



10830

**Flexible porous organic polymers constructed using C(sp<sup>3</sup>)–C(sp<sup>3</sup>) coupling reactions and their high methane-storage capacity**

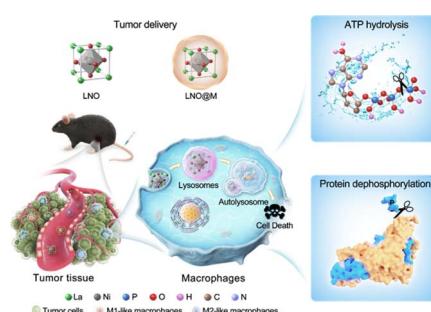
Shuang Zhou, Tianyu Qiu, He Wang, Boyan Tang, Yang Su, Tianhao Nan, Junchao Dong, Zihao Wang, Dongtao Liu\* and Guangshan Zhu\*



10838

**A phosphatase-like nanomaterial promotes autophagy and reprograms macrophages for cancer immunotherapy**

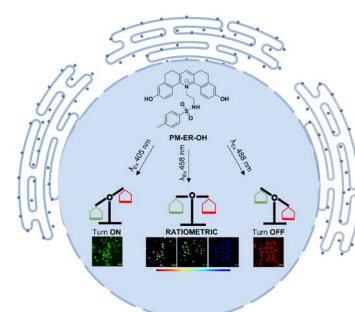
Didar Baimanova, Su Li, Xuejiao J. Gao, Rui Cai, Ke Liu, Junjie Li, Yuchen Liu, Yalin Cong, Xiaoyu Wang, Fen Liu, Qi Li, Guofang Zhang, Hui Wei, Jian Wang, Chunying Chen, Xingfa Gao,\* Yang Li\* and Liming Wang\*



10851

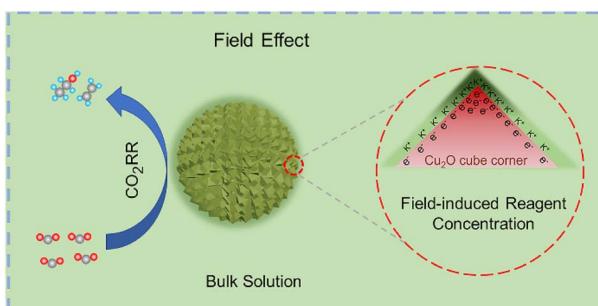
**pH-Assisted multichannel heat shock monitoring in the endoplasmic reticulum with a pyridinium fluorophore**

Sandip Chakraborty, Anivind Kaur Bindra, Anagha Thomas, Yanli Zhao\* and Ayyappanpillai Ajayaghosh\*



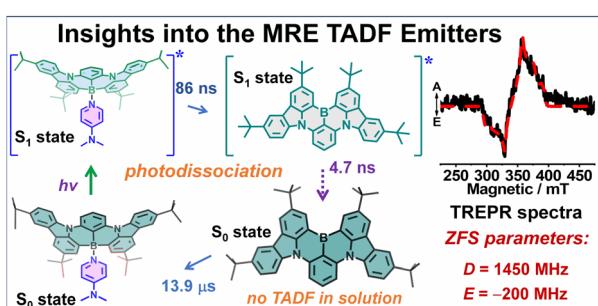
## EDGE ARTICLES

10858


**Enhancing local  $\text{K}^+$  adsorption by high-density cube corners for efficient electroreduction of  $\text{CO}_2$  to  $\text{C}_{2+}$  products**

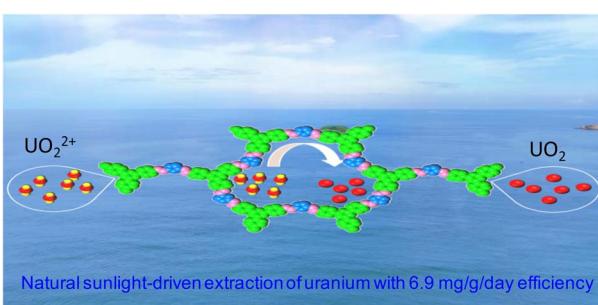
Hu Zang, Changjiang Liu, Qinyuan Ji, Jiahao Wang, Haiyan Lu, Nan Yu and Baoyou Geng\*

10867


**Photophysics and photochemistry of thermally activated delayed fluorescence emitters based on the multiple resonance effect: transient optical and electron paramagnetic resonance studies**

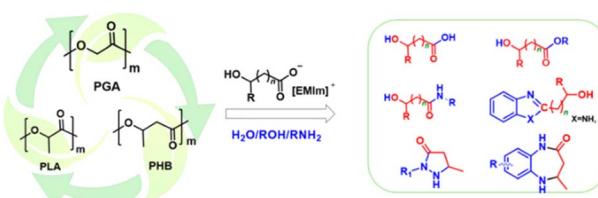
Xi Chen, Lei Sun, Andrey A. Sukhanov, Sandra Doria, Laura Bussotti, Jianzhang Zhao,\* Haijun Xu,\* Bernhard Dick,\* Violeta K. Voronkova\* and Mariangela Di Donato\*

10882


**An imidazole-based covalent-organic framework enabling a super-efficiency in sunlight-driven uranium extraction from seawater**

Lizhen Zhong, Xuefeng Feng,\* Qingyun Zhang, Xianqing Xie and Feng Luo\*

10892


**Hydroxyl carboxylate anion catalyzed depolymerization of biopolymers and transformation to chemicals**

Yanfei Zhao, Hui Zhang, Fengtian Wu,\* Rongxiang Li, Minhao Tang, Yusi Wang, Wei Zeng, Buxing Han and Zhimin Liu\*

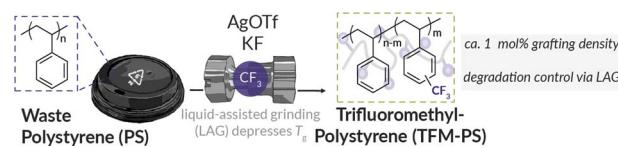


## EDGE ARTICLES

10900

**Liquid-assisted grinding enables a direct mechanochemical functionalization of polystyrene waste**

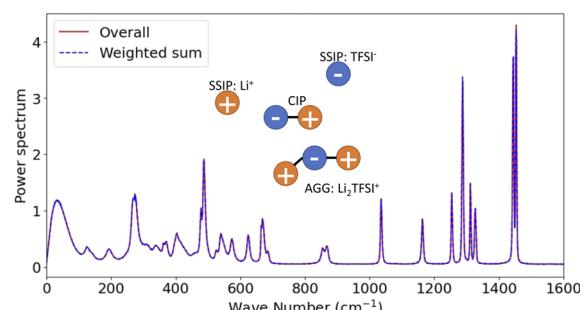
Morgan E. Skala, Sarah M. Zeitler and Matthew R. Golder\*



10908

**Cluster analysis as a tool for quantifying structure–transport properties in simulations of superconcentrated electrolyte**

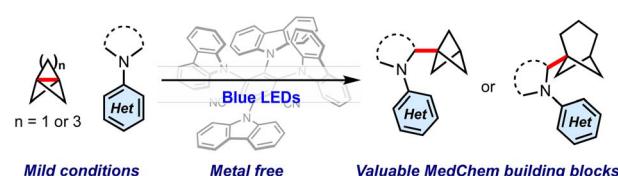
Sheng Bi and Mathieu Salanne\*



10918

**α-Amino bicycloalkylation through organophotoredox catalysis**

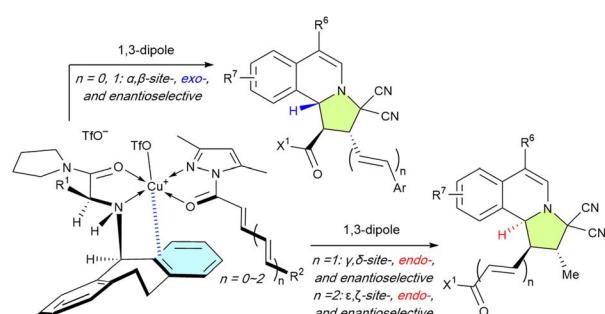
Jeremy Nugent, Adrián López-Francés, Alistair J. Sterling, Min Yi Tay, Nils Frank, James J. Mousseau, Fernanda Duarte\* and Edward A. Anderson\*



10926

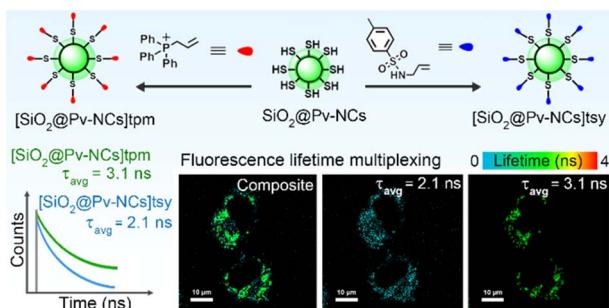
**Chiral  $\pi$ –Cu(II)-catalyzed site-, *exo/endo*-, and enantioselective dearomatic (3 + 2) cycloadditions of isoquinolinium ylides with enamides, dienamides, and a trienamide**

Weiwei Guo, Jianhao Huang and Kazuaki Ishihara\*



## EDGE ARTICLES

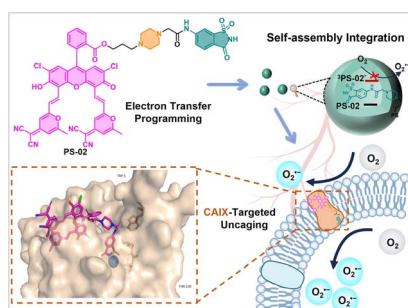
10935



### Surface functionalized perovskite nanocrystals: a design strategy for organelle-specific fluorescence lifetime multiplexing

Anik Kumar Dey, Subhadeep Das, Sharon Mary Jose, Sreejesh Sreedharan, Noufal Kandoth, Surajit Barman, Abhijit Patra,\* Amitava Das\* and Sumit Kumar Pramanik\*

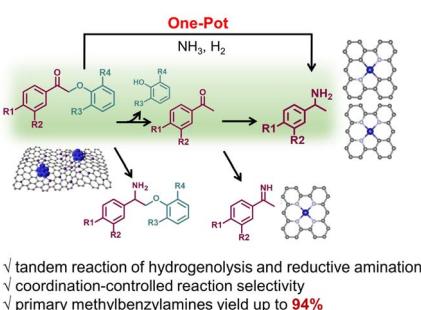
10945



### Self-assembly-integrated tumor targeting and electron transfer programming towards boosting tumor type I photodynamic therapy

Wenlong Chen, Zehui Wang, Gaobo Hong, Jianjun Du, Fengling Song\* and Xiaojun Peng

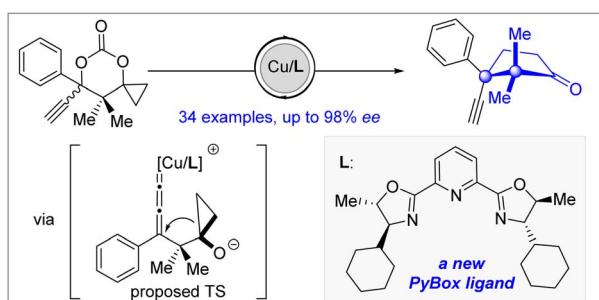
10954



### Atomically dispersed cobalt catalysts for tandem synthesis of primary benzylamines from oxidized $\beta$ -O-4 segments

Sen Luan, Wei Wu, Bingxiao Zheng, Yuxuan Wu, Minghua Dong, Xiaojun Shen, Tianjiao Wang, Zijie Deng, Bin Zhang, Bingfeng Chen, Xueqing Xing, Haihong Wu,\* Huizhen Liu\* and Buxing Han\*

10963



### Catalytic asymmetric intramolecular propargylation of cyclopropanols to access the cuparane core

Yankun Zhao, Hongya Yan, Yulian Zhang, Tao Zhou, Mengxing Tian, Chongzhou Zhang, Shan Yuan, Hanyue Qiu,\* Ling He and Min Zhang\*

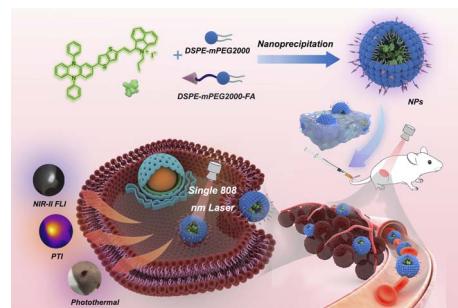


## EDGE ARTICLES

10969

**Dual-modal imaging-guided agent based on NIR-II aggregation-induced emission luminogens with balanced phototheranostic performance**

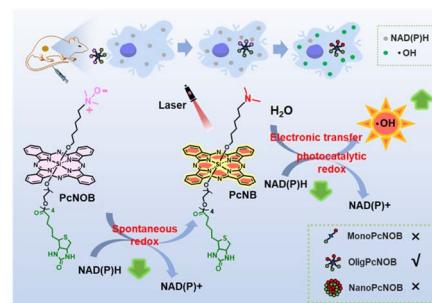
Chengjun Dong, Ziwen Zhang, Hongyu Wu, Xinting Liang, Shihao Pang, Kehuan Wu, Jie Sun, Xuemei Dong, Lixin Sun, Xianfeng Gu\* and Chunchang Zhao\*



10980

**Efficient hydroxyl radical generation of an activatable phthalocyanine photosensitizer: oligomer higher than monomer and nanoaggregate**

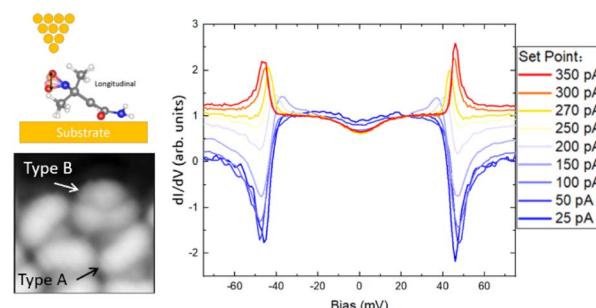
Li Li, Yalan Liao, Shuwen Fu, Zixuan Chen, Tinghe Zhao, Luyue Fang and Xingshu Li\*



10989

**Large negative differential conductance and its transformation in a single radical molecule**

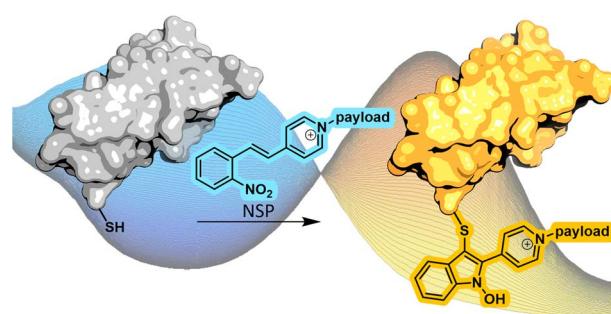
Xiangqian Tang, Wenyu Wang, Haitao Tang, Muyu Wang, Xia Ye, Dong Hao, Jinyu Zhang, Xinyan Shan and Xinghua Lu\*



10997

**NSPs: chromogenic linkers for fast, selective, and irreversible cysteine modification**

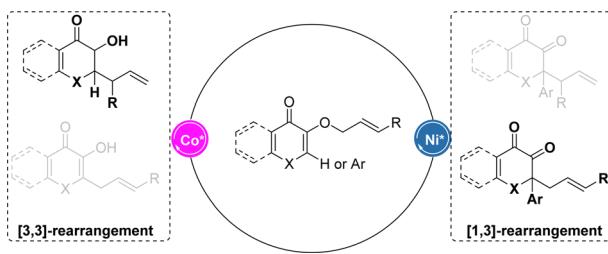
Yong Hua, Zhi Zou, Alessandro Prescimone, Thomas R. Ward, Marcel Mayor and Valentin Köhler\*



## EDGE ARTICLES

11005

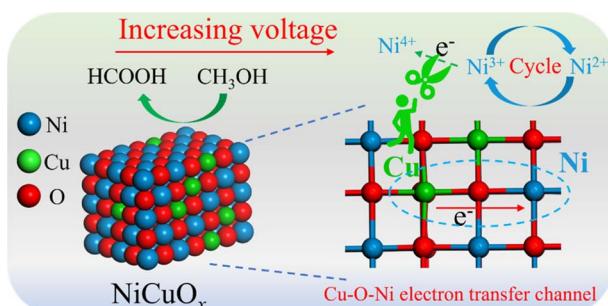
## [1,3]-rearrangement or [3,3]-rearrangement?



## Asymmetric catalytic [1,3]- or [3,3]-sigmatropic rearrangement of 3-allyloxy-4H-chromenones and their analogues

Yi Li, Lichao Ning, Qi Tang, Kexin Lan, Bingqian Yang, Qianchi Lin, Xiaoming Feng\* and Xiaohua Liu\*

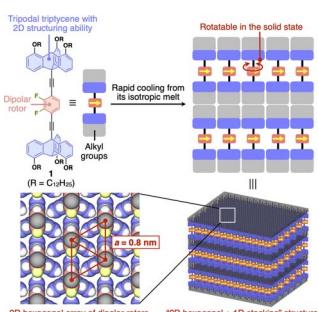
11013



## Construction of an electron-transfer channel via Cu–O–Ni to inhibit the overoxidation of Ni for durable methanol oxidation at industrial current density

Han Tian, Xiaohan Wang, Wenshu Luo, Rundong Ma, Xu Yu, Shujing Li, Fantao Kong, Xiangzhi Cui\* and Jianlin Shi

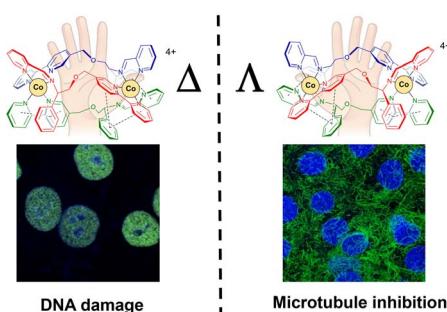
11021



## 2D hexagonal assembly of a dipolar rotor with a close interval of 0.8 nm using a triptycene-based supramolecular scaffold

Takejiro Ogawa, Fumitaka Ishiwari,\* Fatin Hajjaj, Yoshiaki Shoji, Takashi Kajitani, Koji Yazawa, Takahiro Ohkubo and Takanori Fukushima\*

11029



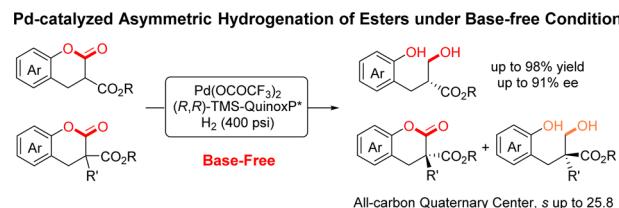
## Dicobalt(II) helices kill colon cancer cells via enantiomer-specific mechanisms: DNA damage or microtubule disruption

Hualong Song,\* Hana Kostrhunova, Jakub Cervinka, Julie Macpherson, Jaroslav Malina, Teena Rajan, Roger Phillips, Miles Postings, Samantha Shepherd, Xuejian Zhang, Viktor Brabec,\* Nicola J. Rogers\* and Peter Scott\*

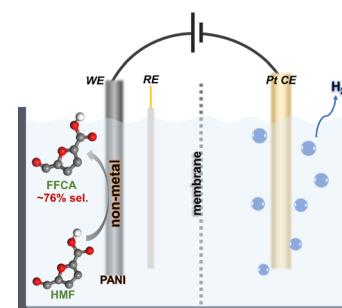


## EDGE ARTICLES

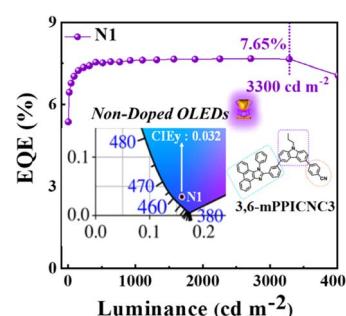
11038

**Palladium-catalyzed asymmetric hydrogenation of lactones under base-free conditions**Han Wang, Shan-Shan Xun, Chang-Bin Yu\*  
and Yong-Gui Zhou\*

11043

**Selective electrooxidation of 5-hydroxymethylfurfural to 5-formyl-furan-2-formic acid on non-metallic polyaniline catalysts: structure–function relationships**Xingyu Lu, Ke Qi, Xueya Dai, Yunlong Li, Di Wang,  
Jing Dou and Wei Qi\*

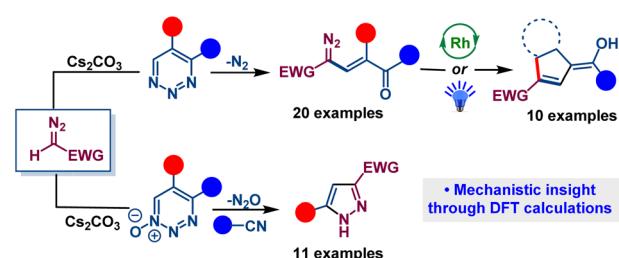
11053

**A record-high EQE of 7.65%@3300 cd m<sup>-2</sup> achieved in non-doped near-ultraviolet OLEDs based on novel D'-D-A type bipolar fluorophores upon molecular configuration engineering**Haoyuan Qi, Danyu Xie, Zexuan Gao, Shengnan Wang,  
Ling Peng, Yuchao Liu, Shian Ying,\* Dongge Ma\*  
and Shouke Yan\*

11065

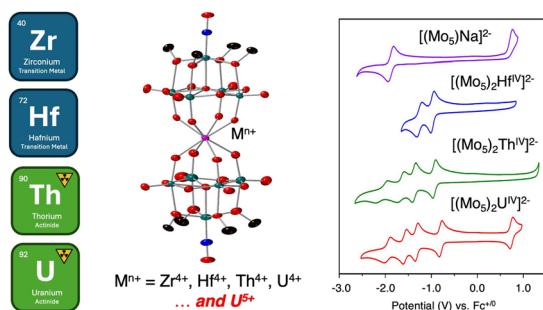
**Denitrogenative dismantling of heteroaromatics by nucleophilic substitution reactions with diazomethyl compounds**

Soumen Biswas, Claire Empel, Luis Mario Sanchez-Palestino, Hadi Arman, Rene M. Koenigs\* and Michael P. Doyle\*

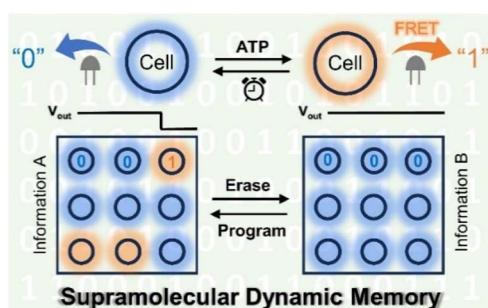


## EDGE ARTICLES

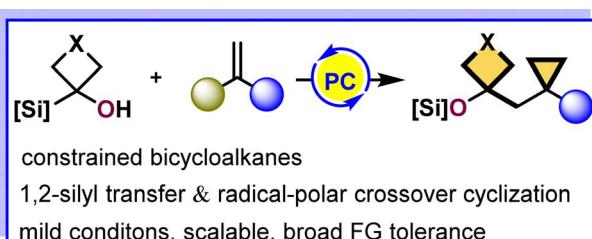
11072



11084



11092



## Leveraging a reduced polyoxomolybdate-alkoxide cluster for the formation of a stable U(v) sandwich complex

Dominic Shiels,\* William W. Brennessel, Matthew R. Crawley and Ellen M. Matson\*

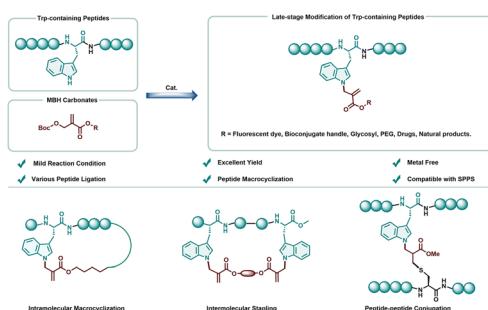
## An enzymolysis-induced energy transfer co-assembled system for spontaneously recoverable supramolecular dynamic memory

Xuanyu Wang, Zhao Gao\* and Wei Tian\*

## Synthesis of constrained bicycloalkanes through bibase-promoted brook rearrangement/radical-polar crossover cyclization

Xinke Ouyang, Bingyao Shi, Yuanyuan Zhao, Zhimin Zhu, Ziyang Li, Yuxin Yang and Chao Shu\*

11099



## Late-stage peptide modification and macrocyclization enabled by tertiary amine catalyzed tryptophan allylation

Yuyang Liu, Guofeng Li, Wen Ma, Guangjun Bao, Yiping Li, Zeyuan He, Zhaoqing Xu,\* Rui Wang\* and Wangsheng Sun\*

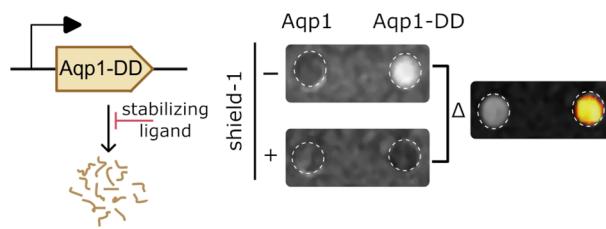


## EDGE ARTICLES

11108

**Destabilized reporters for background-subtracted, chemically-gated, and multiplexed deep-tissue imaging**

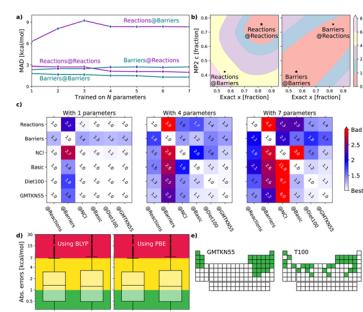
Jason Yun, Yimeng Huang, Austin D. C. Miller, Brandon L. Chang, Logan Baldini, Kaamini M. Dhanabalan, Eugene Li, Honghao Li and Arnab Mukherjee\*



11122

**Identifying and embedding transferability in data-driven representations of chemical space**

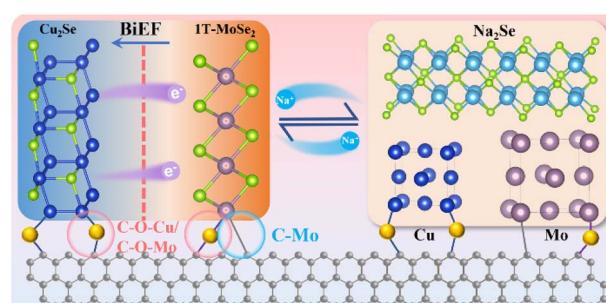
Tim Gould, Bun Chan, Stephen G. Dale and Stefan Vuckovic\*



11134

**A dual heterostructure enables the stabilization of 1T-rich MoSe<sub>2</sub> for enhanced storage of sodium ions**

Yunfeng Chao, Shenghui Jia, Jinzhao Li, Guohui Chen, Lu Liu, Fei Tang, Jianhua Zhu,\* Caiyun Wang\* and Xinwei Cui



## CORRECTIONS

11145

**Correction: Convergent synthesis of thiadiazole dioxides from simple ketones and amines through an unusual nitrogen-migration mechanism**

Kunlayanee Punjajom, Paul P. Sinclair, Ishika Saha, Mark Seierstad, Michael K. Ameriks, Pablo García-Reynaga,\* Terry P. Lebold\* and Richmond Sarpong\*



## CORRECTIONS

11148

**Correction: Investing in entropy: the strategy of cucurbit[*n*]urils to accelerate the intramolecular Diels–Alder cycloaddition reaction of tertiary furfuryl amines**

Karen de la Vega-Hernández, Marcos G. Suero\* and Pablo Ballester\*

