

# Chemical Science

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## IN THIS ISSUE

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**Cover**  
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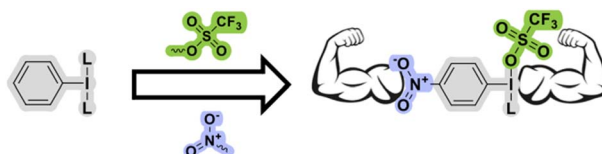
**Inside cover**  
See Na Wang, Hongxun Hao *et al.*, pp. 3800–3830. Image reproduced by permission of Xiongtao Ji, Na Wang, Jingkang Wang, Ting Wang, Xin Huang and Hongxun Hao from *Chem. Sci.*, 2024, 15, 3800.

## PERSPECTIVE

3784

### A decade of lessons in the activation of ArL<sub>2</sub> species

Tania, Marcus Sceney and Jason L. Dutton\*

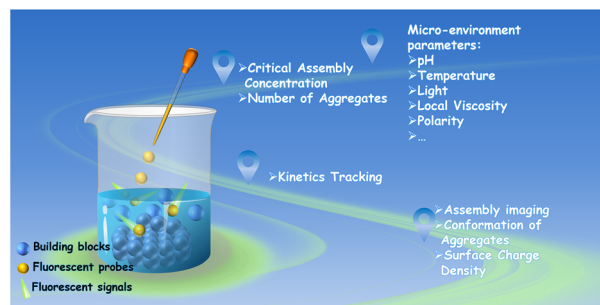


## REVIEWS

3800

### Non-destructive real-time monitoring and investigation of the self-assembly process using fluorescent probes

Xiongtao Ji, Na Wang,\* Jingkang Wang, Ting Wang, Xin Huang and Hongxun Hao\*



# EES Catalysis

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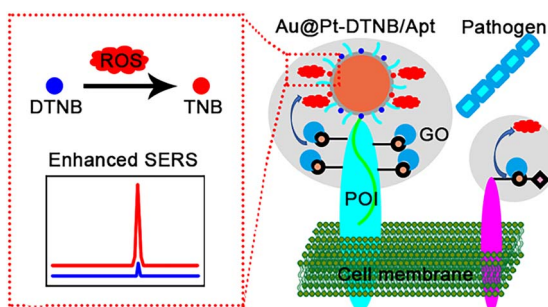
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Fundamental questions  
Elemental answers



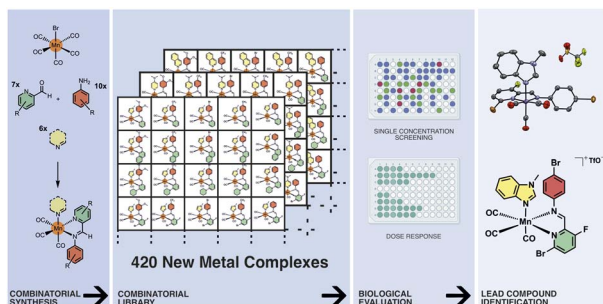
3901



### In situ SERS imaging of protein-specific glycan oxidation on living cells to quantitatively visualize pathogen–cell interactions

Yuru Wang, Shan Wu, Yuanjiao Yang, Yuhui Yang, Huipu Liu, Yunlong Chen\* and Huangxian Ju\*

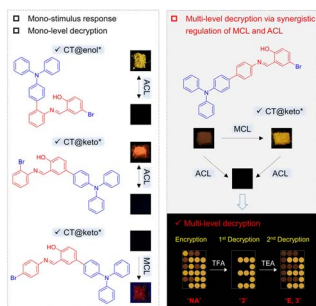
3907



### Discovery of antibacterial manganese(i) tricarbonyl complexes through combinatorial chemistry

Mirco Scaccaglia, Michael P. Birbaumer, Silvana Pinelli, Giorgio Pelosi and Angelo Frei\*

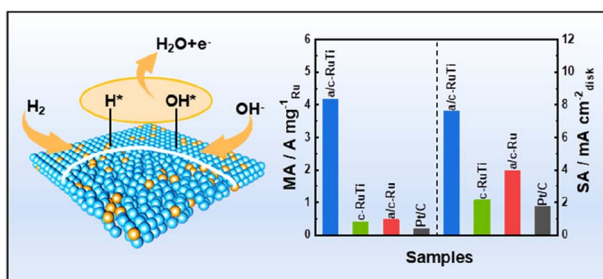
3920



### Multi-site isomerization of synergistically regulated stimuli-responsive AIE materials toward multi-level decryption

Weiren Zhong, Jianyu Zhang, Yuting Lin, Shouji Li, Yalan Yang, Wen-Jin Wang, Chuanling Si,\* Fritz E. Kühn, Zheng Zhao, Xu-Min Cai\* and Ben Zhong Tang\*

3928



### Amorphous–crystalline RuTi nanosheets enhancing OH species adsorption for efficient hydrogen oxidation catalysis

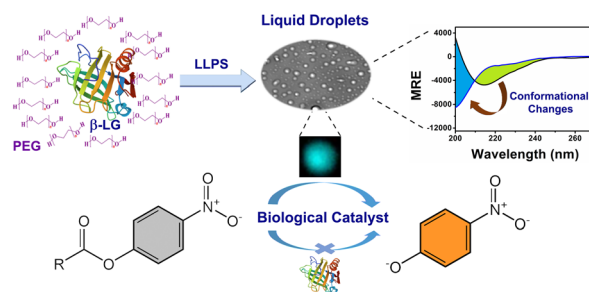
Licheng Wei, Nan Fang, Fei Xue, Shangheng Liu, Wei-Hsiang Huang, Chih-Wen Pao, Zhiwei Hu, Yong Xu,\* Hongbo Geng\* and Xiaoqing Huang\*



3936

### Deciphering the liquid–liquid phase separation induced modulation in the structure, dynamics, and enzymatic activity of an ordered protein $\beta$ -lactoglobulin

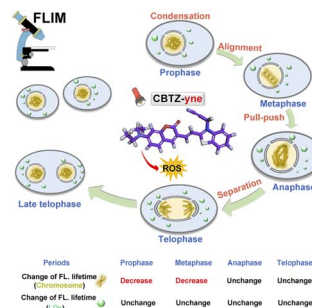
Saurabh Rai, Srikrishna Pramanik and Saptarshi Mukherjee\*



3949

### Precisely modulating the chromatin tracker via substituent engineering: reporting pathological oxidative stress during mitosis

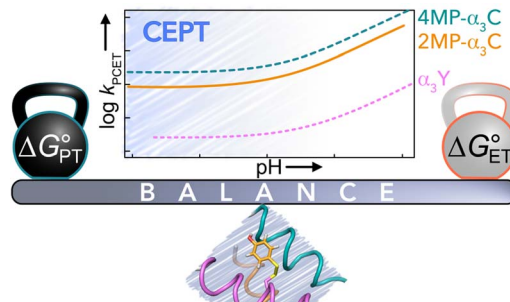
Jinsong Li, Yingyong Ni, Junjun Wang,\* Yicai Zhu, Aidong Wang, Xiaojiao Zhu, Xianshun Sun, Sen Wang, Dandan Li and Hongping Zhou\*



3957

### Switching the proton-coupled electron transfer mechanism for non-canonical tyrosine residues in a *de novo* protein

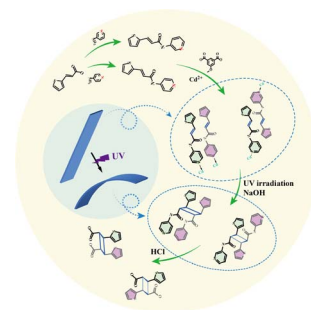
Astrid Nilsen-Moe, Clorice R. Reinhardt, Ping Huang, Hemlata Agarwala, Rosana Lopes, Mauricio Lasagna, Starla Glover, Sharon Hammes-Schiffer, Cecilia Tommos\* and Leif Hammarström\*



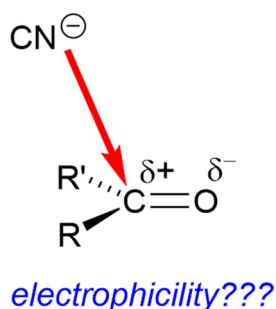
3971

### [2 + 2] cycloaddition and its photomechanical effects on 1D coordination polymers with reversible amide bonds and coordination site regulation

Lei Wang, Si-Bo Qiao, Yan-Ting Chen, Xun Ma, Wei-Ming Wei, Jun Zhang, Lin Du\* and Qi-Hua Zhao\*

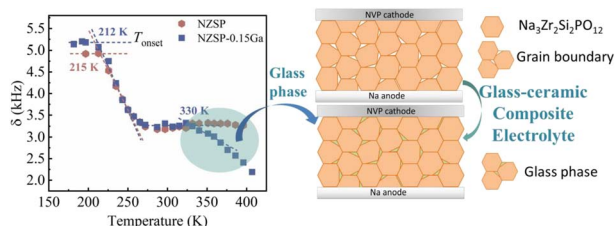


3980

**What defines electrophilicity in carbonyl compounds**

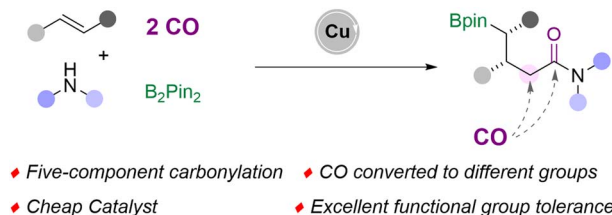
F. Matthias Bickelhaupt\* and Israel Fernández\*

3988

**The glass phase in the grain boundary of  $\text{Na}_3\text{Zr}_2\text{Si}_2\text{PO}_{12}$ , created by gallium modulation**

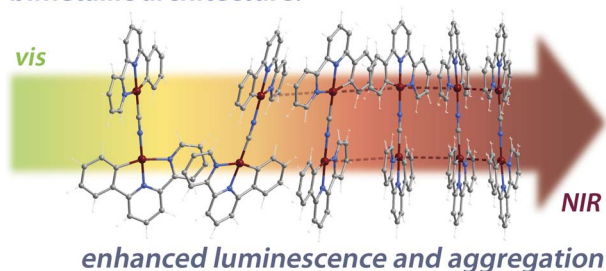
Chenjie Lou, Wenda Zhang, Jie Liu, Yanan Gao, Xuan Sun, Jipeng Fu, Yongchao Shi, Ligang Xu, Huajie Luo, Yongjin Chen, Xiang Gao, Xiaojun Kuang, Lei Su and Mingxue Tang\*

3996

**Copper-catalyzed carbonylative multi-component borylamidation of alkenes for synthesizing  $\gamma$ -boryl amides with CO as both methylene and carbonyl sources**

Hui-Qing Geng, Yan-Hua Zhao, Peng Yang and Xiao-Feng Wu\*

4005

**bimetallic architecture:****Cyano-bridged diplatinum(II) complexes: ligand and solvent effect on aggregation and luminescence**

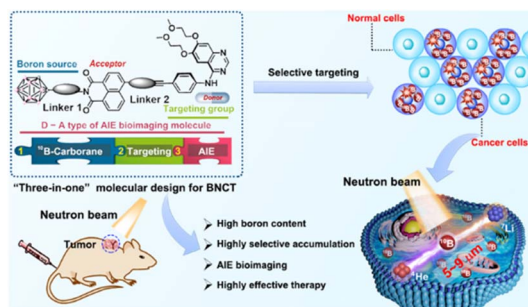
Viktoria V. Khistiaeva, Stefan Buss, Toni Eskelinen, Pipsa Hirva, Niko Kinnunen, Joshua Friedel, Lukas Kletsch, Axel Klein,\* Cristian A. Strassert\* and Igor O. Koshevoy\*



4019

## Molecular engineering of AIE-active boron clustoluminogens for enhanced boron neutron capture therapy

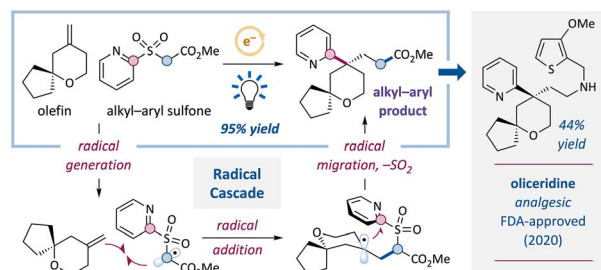
Wenli Ma, Yanyang Wang, Yilin Xue, Mengmeng Wang, Changsheng Lu, Wanhua Guo, Yuan-Hao Liu, Diyun Shu, Guoqiang Shao, Qinfeng Xu,\* Deshuang Tu\* and Hong Yan\*



4031

## A free-radical design featuring an intramolecular migration for a synthetically versatile alkyl-(hetero) arylation of simple olefins

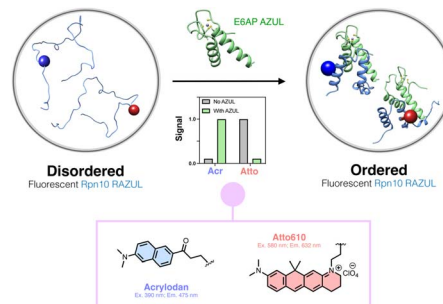
Dylan J. Babcock, Andrew J. Wolfram, Jaxon L. Barney, Santino M. Servagno, Ayush Sharma and Eric D. Nacsá\*



4041

## High-throughput assay exploiting disorder-to-order conformational switches: application to the proteasomal Rpn10:E6AP complex

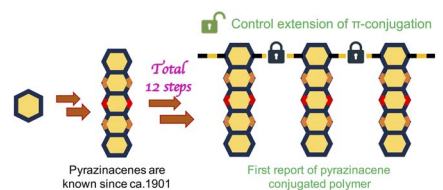
Christine S. Muli, Sergey G. Tarasov and Kylie J. Walters\*



4054

## Pyrazinacene conjugated polymers: a breakthrough in synthesis and unraveling the conjugation continuum

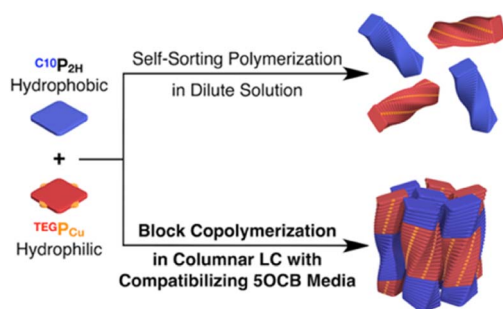
Fatima Hameed, Arindam Maity, Victor S. Francis and Nagarjuna Gavvalapalli\*



- ✓ A series of 4 polymers are generated at RT in a few minutes
- ✓ Challenges strict stoichiometric balance-  
High DP realized at non-equivalent monomer ratios
- ✓ Redox state of pyrazine controls conjugation between repeat units
- ✓ Polymerization lowers LUMO level by ca. 2 eV compared to monomer
- ✓ LUMO level is (-4.5 eV) in the range of best n-type polymers
- ✓ Polymers exhibit ionochromism



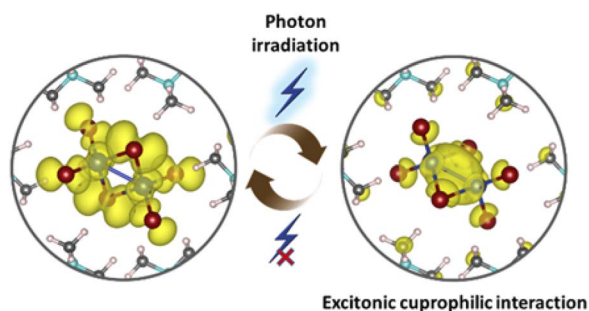
4068



### Supramolecular copolymerization of hydrophobic and hydrophilic monomers in liquid crystalline media

Daiki Morishita, Yoshimitsu Itoh,\* Ko Furukawa, Noriyoshi Arai, Xu-Jie Zhang and Takuzo Aida\*

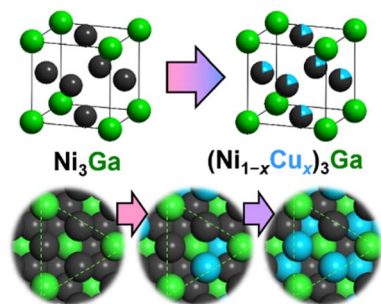
4075



### Excitonic cuprophilic interactions in one-dimensional hybrid organic-inorganic crystals

Nahid Hassan, Suneetha Nagaraja, Sauvik Saha, Kartick Tarafder and Nirmalya Ballav\*

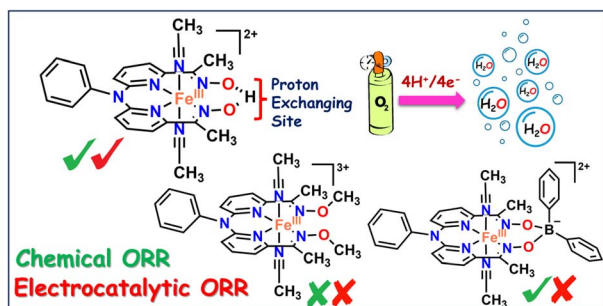
4086



### Active site tuning based on pseudo-binary alloys for low-temperature acetylene semihydrogenation

Jiamin Ma, Feilong Xing, Ken-ichi Shimizu and Shinya Furukawa\*

4095



### Catalytic reduction of oxygen to water by non-heme iron complexes: exploring the effect of the secondary coordination sphere proton exchanging site

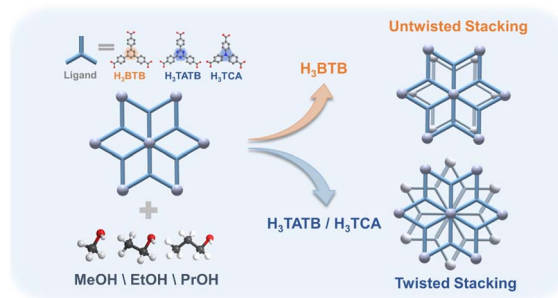
Aakash Santra, Avijit Das, Simarjeet Kaur, Priya Jain, Pravin P. Ingole and Sayantan Paria\*



4106

### Polar alcohol guest molecules regulate the stacking modes of 2-D MOF nanosheets

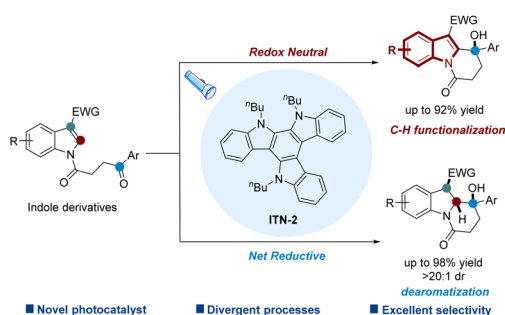
Yue Cheng, Wen-Qi Tang, Lu-Ting Geng, Ming Xu, Jian-Ping Zhu, Sha-Sha Meng and Zhi-Yuan Gu\*



4114

### Tunable C–H functionalization and dearomatization enabled by an organic photocatalyst

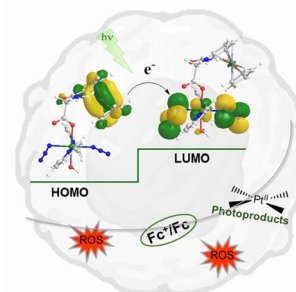
Bohang An, Hao Cui, Chao Zheng,\* Ji-Lin Chen, Feng Lan, Shu-Li You\* and Xiao Zhang\*



4121

### Tuning the photoactivated anticancer activity of Pt(IV) compounds via distant ferrocene conjugation

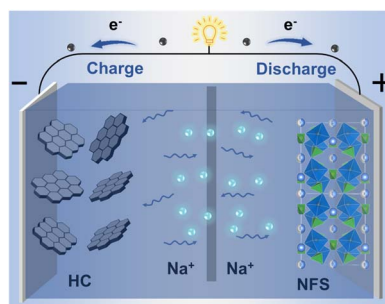
Huayun Shi, Fortuna Ponte, Jaspreet S. Grewal, Guy J. Clarkson, Cinzia Imberti, Ian Hands-Portman, Robert Dallmann, Emilia Sicilia\* and Peter J. Sadler\*



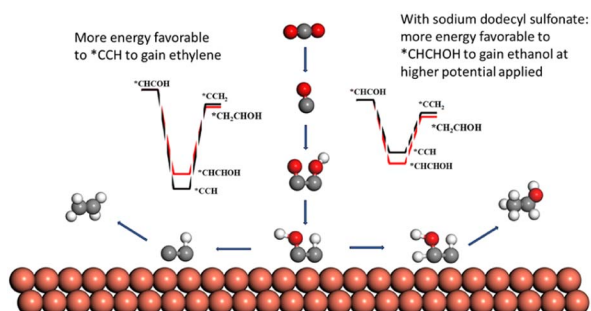
4135

### Revealing the effect of conductive carbon materials on the sodium storage performance of sodium iron sulfate

Wenqing Zhu, Zhiqiang Hao, Xiaoyan Shi, Xunzhu Zhou, Zhuo Yang, Lingling Zhang, Zongcheng Miao,\* Lin Li\* and Shu-Lei Chou\*



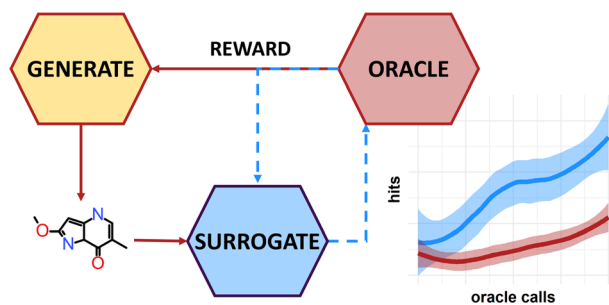
4140



### Alkyl sulfonate surfactant mediates electroreduction of carbon dioxide to ethylene or ethanol over hydroxide-derived copper catalysts

Yiding Wang, Runyao Zhao, Yunpeng Liu, Fengtao Zhang, Yuepeng Wang, Zhonghua Wu, Buxing Han and Zhimin Liu\*

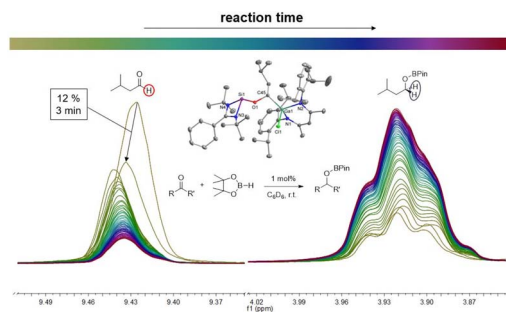
4146



### Sample efficient reinforcement learning with active learning for molecular design

Michael Dodds, Jeff Guo, Thomas Löhner, Alessandro Tibo, Ola Engkvist and Jon Paul Janet\*

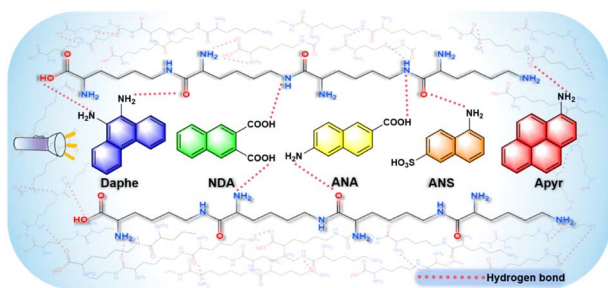
4161



### Catalytic hydroboration of aldehydes and ketones with an electron-rich acyclic metallasilylene

Leon Kapp, Christoph Wölper, Hannah Siera, Gebhard Haberhauer\* and Stephan Schulz\*

4171



### $\epsilon$ -Polylysine organic ultra-long room-temperature phosphorescent materials based on phosphorescent molecule doping

Jiaying Cui, Syed Husnain Ali, Zhuoyao Shen, Wensheng Xu, Jiayi Liu, Pengxiang Li, Yang Li,\* Ligong Chen and Bowei Wang\*



4179

**Rule breaker boron clusters: a new class of hypoelectronic osmaborane clusters [(Cp\*Os)<sub>2</sub>B<sub>n</sub>H<sub>n</sub>] (*n* = 6–10)**

Ketaki Kar, Sourav Kar and Sundargopal Ghosh\*

