

# Chemical Science

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## IN THIS ISSUE

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**Cover**  
See Jake L. Greenfield *et al.*, pp. 3872–3878. Image reproduced by permission of Jake Greenfield from *Chem. Sci.*, 2024, 15, 3872.



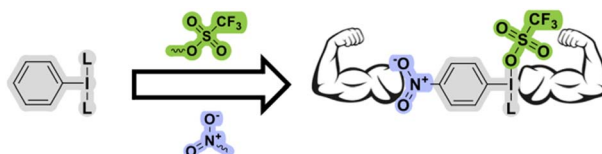
**Inside cover**  
See Na Wang, Hongxun Hao *et al.*, pp. 3800–3830. Image reproduced by permission of Xiongtao Ji, Na Wang, Jingkang Wang, Ting Wang, Xin Huang and Hongxun Hao from *Chem. Sci.*, 2024, 15, 3800.

## PERSPECTIVE

3784

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

Tania, Marcus Sceney and Jason L. Dutton\*

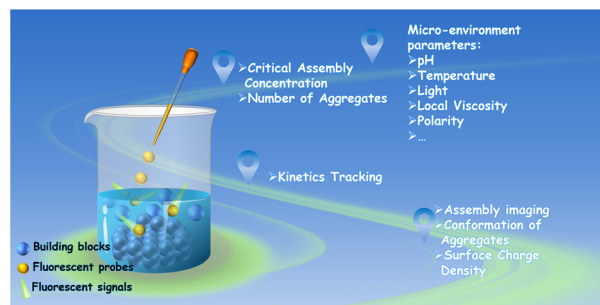


## REVIEWS

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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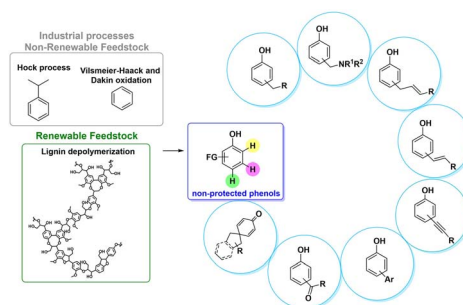
Fundamental questions  
Elemental answers

## REVIEWS

3831

### Csp<sup>2</sup>-H functionalization of phenols: an effective access route to valuable materials via Csp<sup>2</sup>-C bond formation

Giulia Brufani, Benedetta Di Erasmo, Chao-Jun Li and Luigi Vaccaro\*

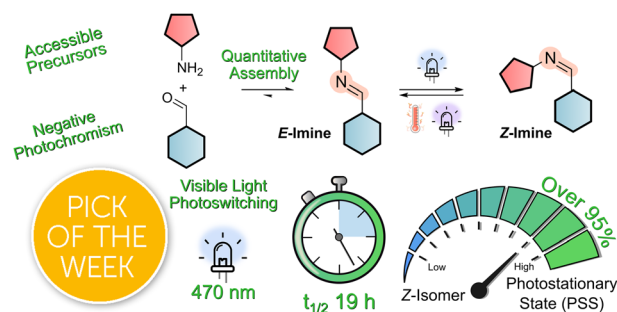


## EDGE ARTICLES

3872

### Photoswitchable imines: aryliminopyrazoles quantitatively convert to long-lived Z-isomers with visible light

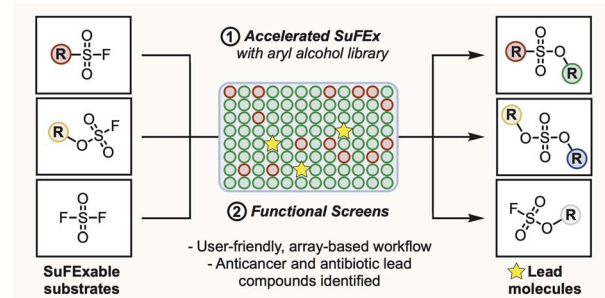
Jiarong Wu, Lasse Kreimendahl, Suyuan Tao, Olga Anhalt and Jake L. Greenfield\*



3879

### Modular synthesis of functional libraries by accelerated SuFEx click chemistry

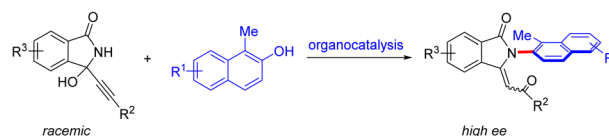
Joshua A. Homer, Rebecca A. Koelln, Andrew S. Barrow, Timothy L. Gialelis, Zlata Boiarska, Nikita S. Steinohrt, Erinna F. Lee, Wen-Hsuan Yang, Robert M. Johnson, Taemoon Chung, Amber N. Habowski, Dharmendra S. Vishwakarma, Debmalya Bhunia, Charlotte Avanzi, Adam D. Moorhouse, Mary Jackson, David A. Tuveson, Scott K. Lyons, Michael J. Lukey, W. Douglas Fairlie, Shozeb M. Haider, Michel O. Steinmetz, Andrea E. Prota and John E. Moses\*



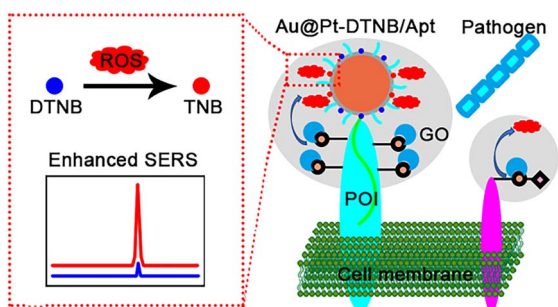
3893

### Organocatalytic enantioselective synthesis of C<sub>sp2</sub>-N atropisomers via formal C<sub>sp2</sub>-O bond amination

Chenxiao Qian, Jing Huang, Tingting Huang, Lijuan Song, Jianwei Sun\* and Pengfei Li\*



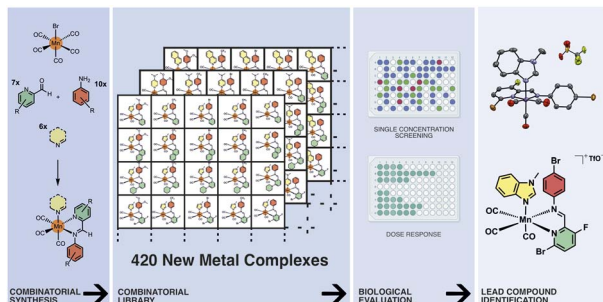
3901



### *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\*

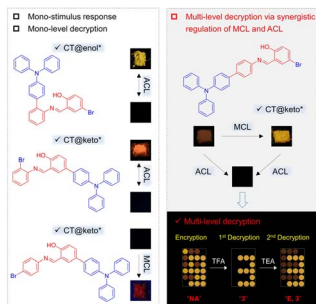
3907



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

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

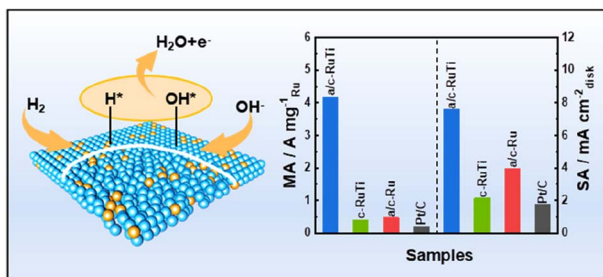
3920



### 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

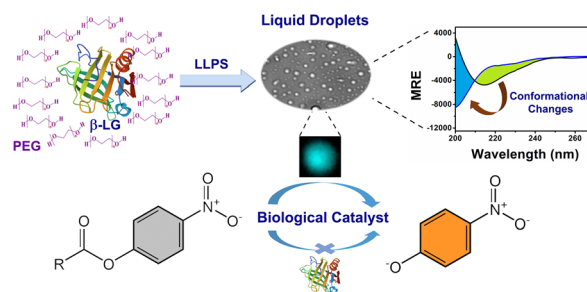
Licheng Wei, Nan Fang, Fei Xue, Shangheng Liu, Wei-Hsiang Huang, Chih-Wen Pao, Zhiwei Hu, Yong Xu,\* Hongbo Geng\* and Xiaoqing Huang\*



3936

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

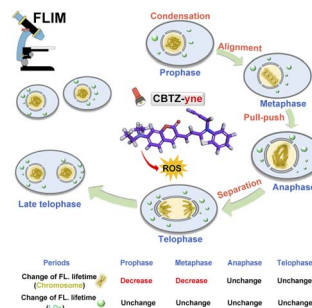
Saurabh Rai, Srikrishna Pramanik and Saptarshi Mukherjee\*



3949

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

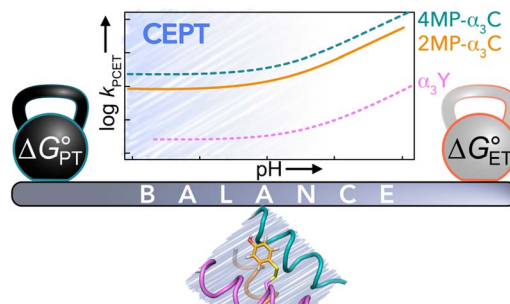
Jinsong Li, Yingyong Ni, Junjun Wang,\* Yicai Zhu, Aidong Wang, Xiaojiao Zhu, Xianshun Sun, Sen Wang, Dandan Li and Hongping Zhou\*



3957

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

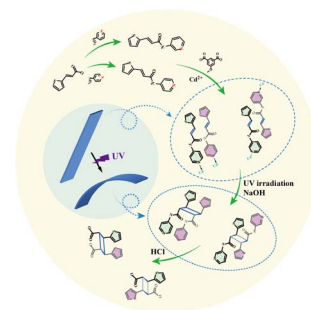
Astrid Nilsen-Moe, Clorice R. Reinhardt, Ping Huang, Hemlata Agarwala, Rosana Lopes, Mauricio Lasagna, Starla Glover, Sharon Hammes-Schiffer, Cecilia Tommos\* and Leif Hammarström\*



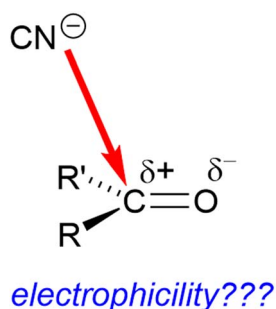
3971

### [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\*

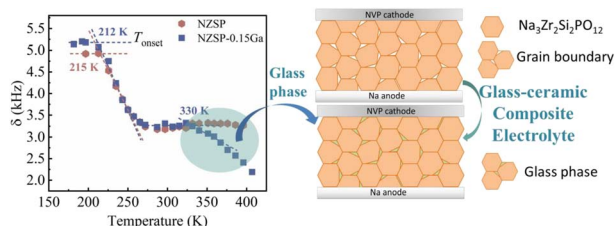


3980

**What defines electrophilicity in carbonyl compounds**

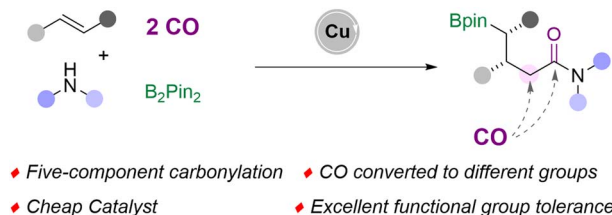
F. Matthias Bickelhaupt\* and Israel Fernández\*

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**

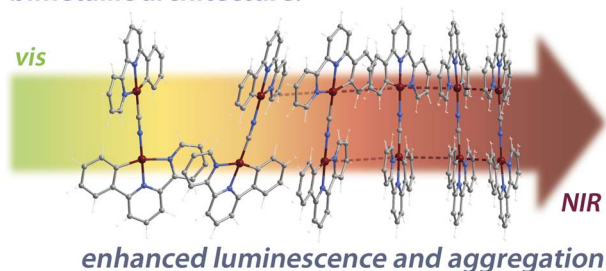
Chenjie Lou, Wenda Zhang, Jie Liu, Yanan Gao, Xuan Sun, Jipeng Fu, Yongchao Shi, Ligang Xu, Huajie Luo, Yongjin Chen, Xiang Gao, Xiaojun Kuang, Lei Su and Mingxue Tang\*

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

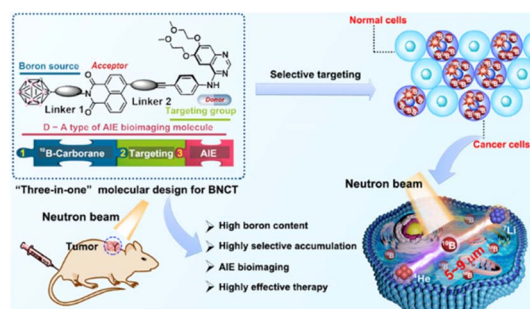
Viktoria V. Khistiaeva, Stefan Buss, Toni Eskelinen, Pipsa Hirva, Niko Kinnunen, Joshua Friedel, Lukas Kletsch, Axel Klein,\* Cristian A. Strassert\* and Igor O. Koshevoy\*



4019

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

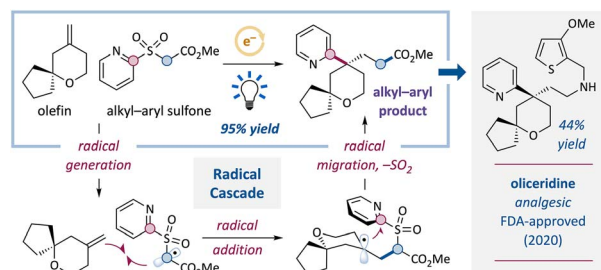
Wenli Ma, Yanyang Wang, Yilin Xue, Mengmeng Wang, Changsheng Lu, Wanhua Guo, Yuan-Hao Liu, Diyun Shu, Guoqiang Shao, Qinfeng Xu,\* Deshuang Tu\* and Hong Yan\*



4031

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

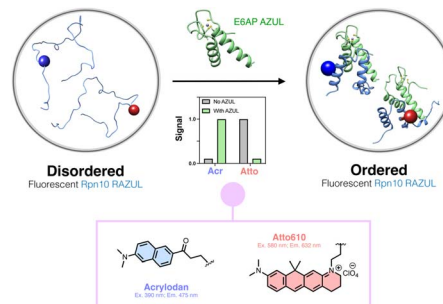
Dylan J. Babcock, Andrew J. Wolfram, Jaxon L. Barney, Santino M. Servagno, Ayush Sharma and Eric D. Nacsá\*



4041

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

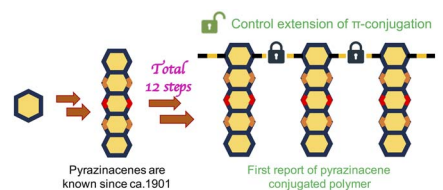
Christine S. Muli, Sergey G. Tarasov and Kylie J. Walters\*



4054

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

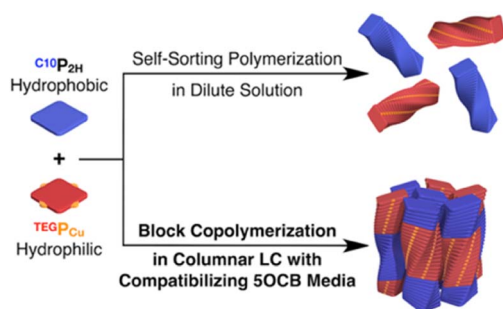
Fatima Hameed, Arindam Maity, Victor S. Francis and Nagarjuna Gavvalapalli\*



- ✓ 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



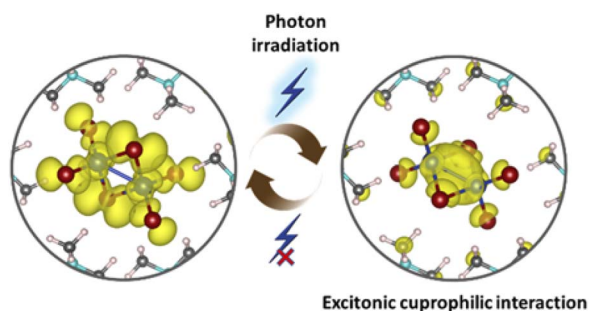
4068



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

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

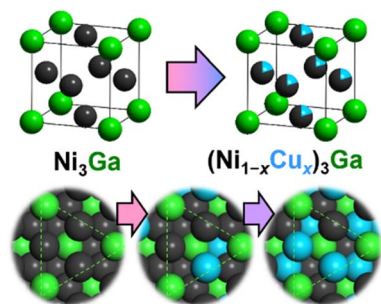
4075



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

Nahid Hassan, Suneetha Nagaraja, Sauvik Saha, Kartick Tarafder and Nirmalya Ballav<sup>\*</sup>

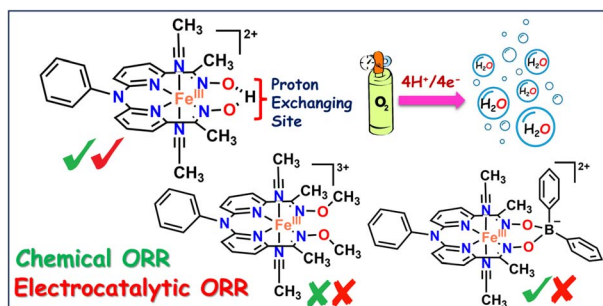
4086



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

Jiamin Ma, Feilong Xing, Ken-ichi Shimizu and Shinya Furukawa<sup>\*</sup>

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<sup>\*</sup>

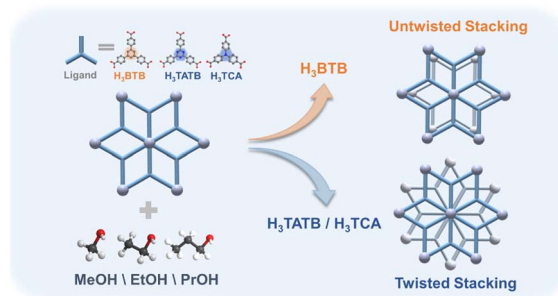




4106

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

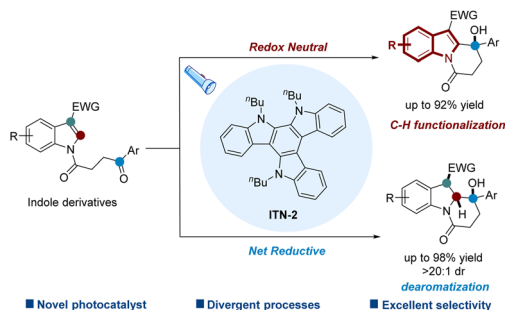
Yue Cheng, Wen-Qi Tang, Lu-Ting Geng, Ming Xu, Jian-Ping Zhu, Sha-Sha Meng and Zhi-Yuan Gu\*



4114

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

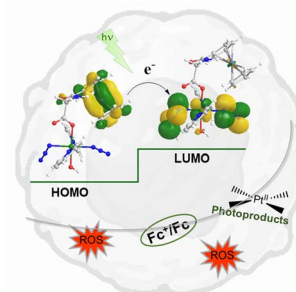
Bohang An, Hao Cui, Chao Zheng,\* Ji-Lin Chen, Feng Lan, Shu-Li You\* and Xiao Zhang\*



4121

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

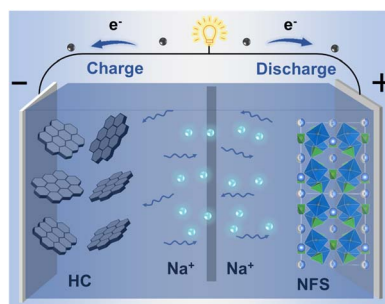
Huayun Shi, Fortuna Ponte, Jaspreet S. Grewal, Guy J. Clarkson, Cinzia Imberti, Ian Hands-Portman, Robert Dallmann, Emilia Sicilia\* and Peter J. Sadler\*



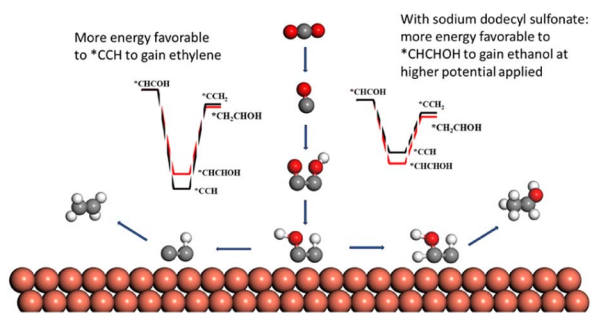
4135

### 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\*



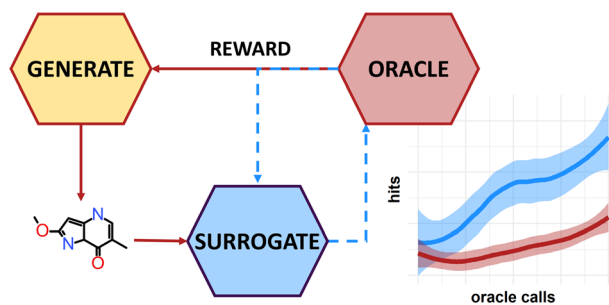
4140



### 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\*

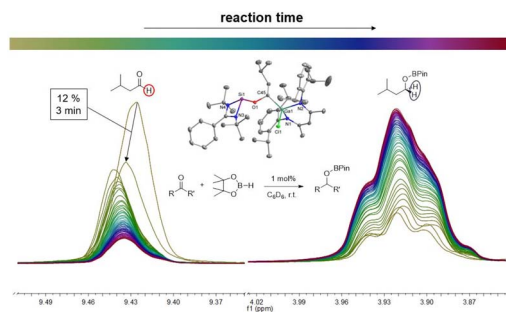
4146



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

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

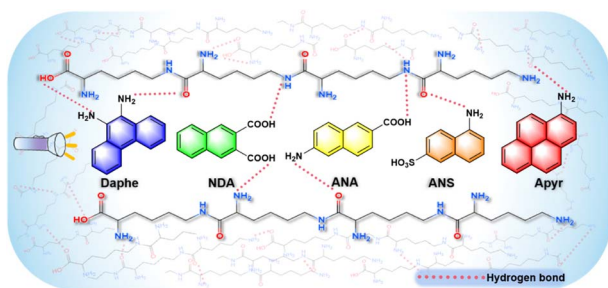
4161



### 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\*

