

Chemical Science

rsc.li/chemical-science

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(11) 3771–4188 (2024)



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 ArIL_2 species

Tania, Marcus Sceney and Jason L. Dutton*

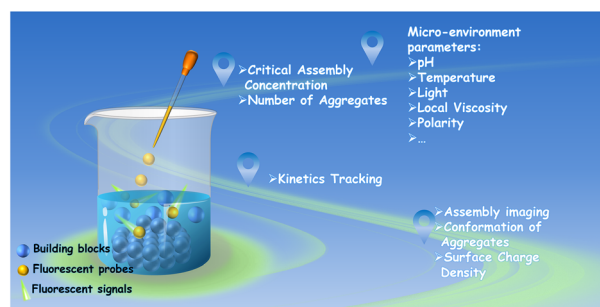


REVIEWS

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

GOLD
OPEN
ACCESS

**Exceptional research on energy
and environmental catalysis**

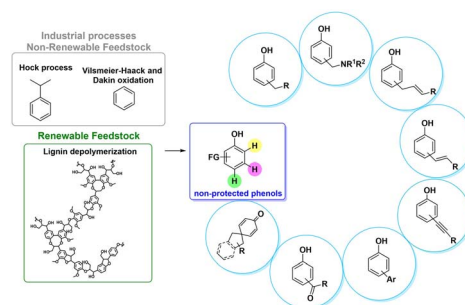
Open to everyone. Impactful for all

rsc.li/EESCatalysis

**Fundamental questions
Elemental answers**

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

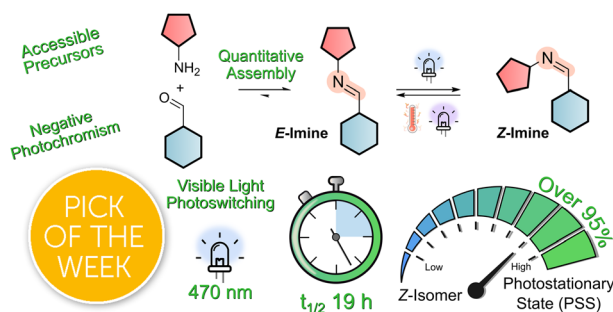
Giulia Brufani, Benedetta Di Erasmo, Chao-Jun Li
and Luigi Vaccaro*



3872

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

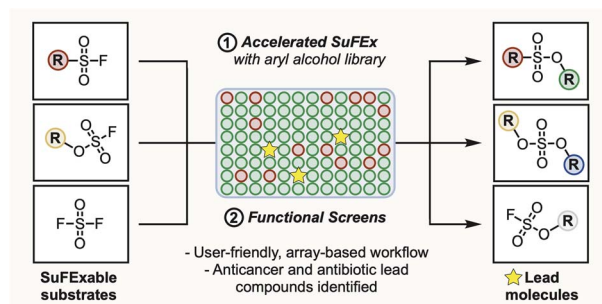
Jiarong Wu, Lasse Kreimendahl, Suyuan Tao, Olga Anhalt
and Jake L. Greenfield*



3879

Joshua A. Homer, Rebecca A. Koelln, Andrew S. Barrow,
Timothy L. Gialelis, Zlata Bojarska, Nikita S. Steinhart,
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*

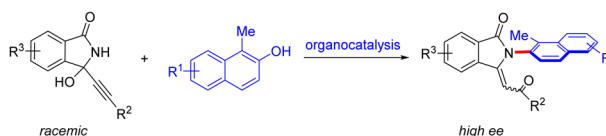
Joshua A. Homer, Rebecca A. Koelln, Andrew S. Barrow,
Timothy L. Gialelis, Zlata Bojarska, Nikita S. Steinhart,
Erinna F. Lee, Wen-Hsuan Yang, Robert M. Johnson,
Taemoon Chung, Amber N. Habowski, Dharmendra
S. Vishwakarma, Debmalya Bhunia, Charlotte Avanzi,
Adam D. Moorhouse, Mary Jackson, David A. Tuveson,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



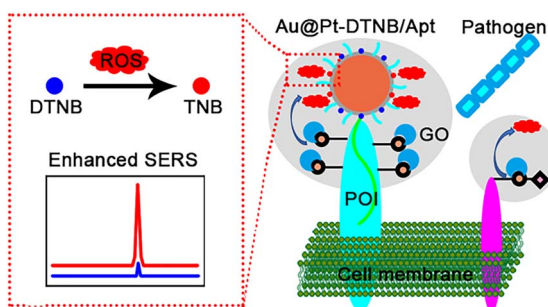
3893

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

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



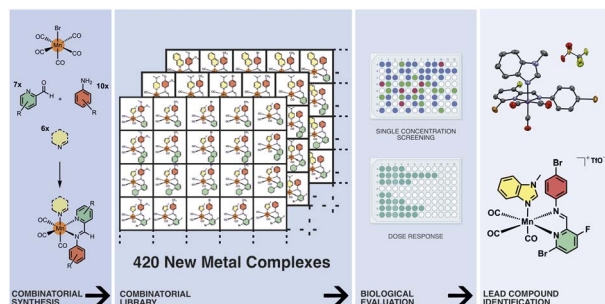
3901



***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*

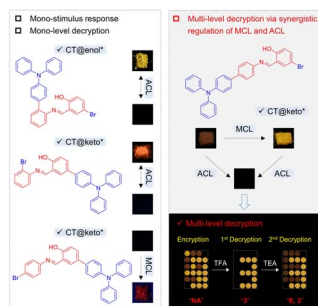
3907



Discovery of antibacterial manganese(I) tricarbonyl complexes through combinatorial chemistry

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

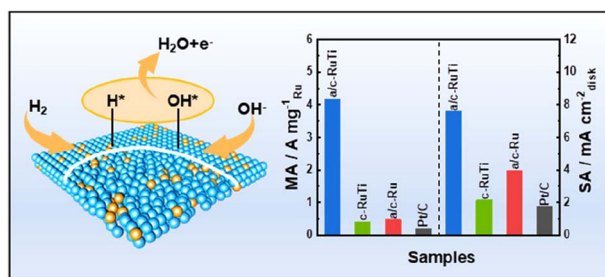
3920



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

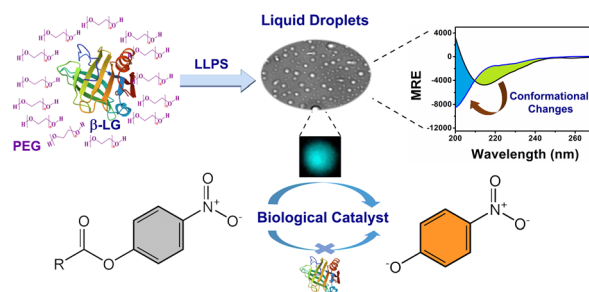
Licheng Wei, Nan Fang, Fei Xue, Shangheng Liu, Wei-Hsiang Huang, Chih-Wen Pao, Zhiwei Hu, Yong Xu,* Hongbo Geng* and Xiaoqing Huang*



3936

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

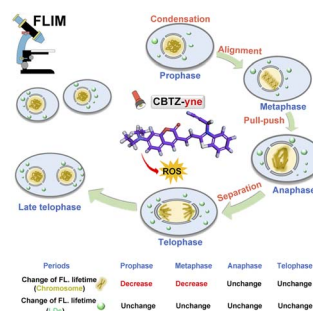
Saurabh Rai, Srikrishna Pramanik and Saptarshi Mukherjee*



3949

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

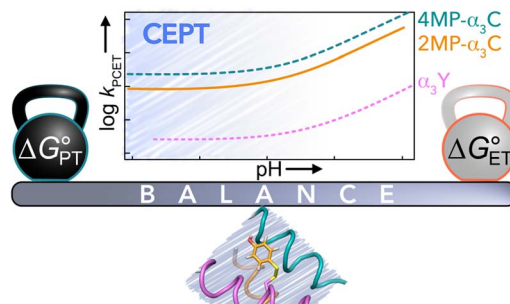
Jinsong Li, Yingyong Ni, Junjun Wang,* Yicai Zhu, Aidong Wang, Xiaojiao Zhu, Xianshun Sun, Sen Wang, Dandan Li and Hongping Zhou*



3957

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

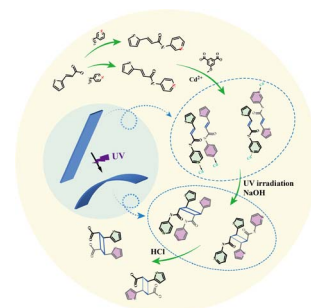
Astrid Nilsen-Moe, Clorice R. Reinhardt, Ping Huang, Hemlata Agarwala, Rosana Lopes, Mauricio Lasagna, Starla Glover, Sharon Hammes-Schiffer, Cecilia Tommos* and Leif Hammarström*



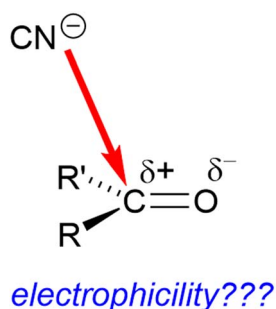
3971

[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*

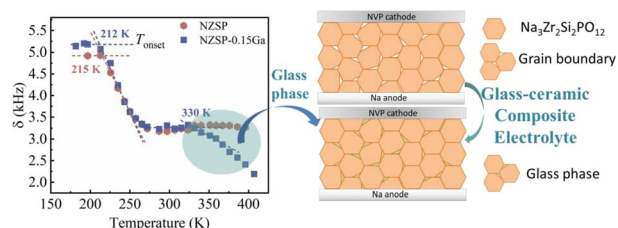


3980

**What defines electrophilicity in carbonyl compounds**

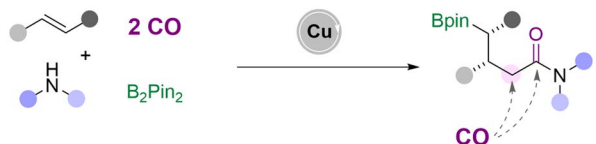
F. Matthias Bickelhaupt* and Israel Fernández*

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

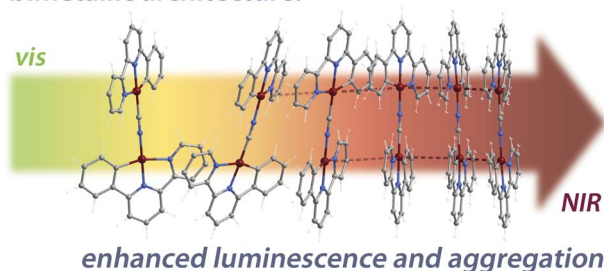


- ♦ Five-component carbonylation ♦ CO converted to different groups
- ♦ Cheap Catalyst ♦ Excellent functional group tolerance

Copper-catalyzed carbonylative multi-component borylamidation of alkenes for synthesizing γ -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**

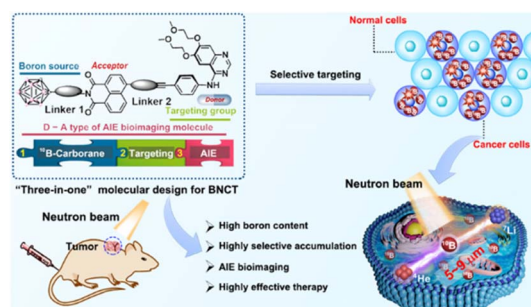
Viktoria V. Khistiaeva, Stefan Buss, Toni Eskelinen, Pipsa Hirva, Niko Kinnunen, Joshua Friedel, Lukas Kletsch, Axel Klein,* Cristian A. Strassert* and Igor O. Koshevoy*



4019

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

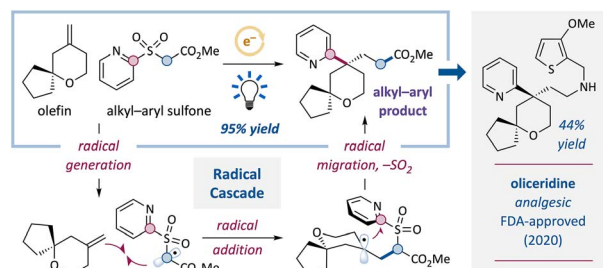
Wenli Ma, Yanyang Wang, Yilin Xue, Mengmeng Wang, Changsheng Lu, Wanhua Guo, Yuan-Hao Liu, Diyun Shu, Guoqiang Shao, Qinfeng Xu,* Deshuang Tu* and Hong Yan*



4031

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

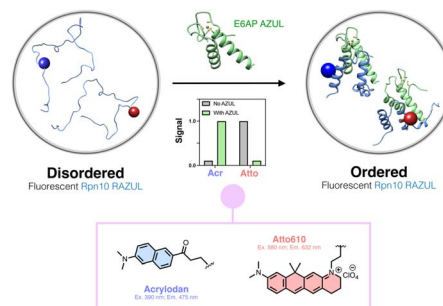
Dylan J. Babcock, Andrew J. Wolfram, Jaxon L. Barney, Santino M. Servagno, Ayush Sharma and Eric D. Nacsa*



4041

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

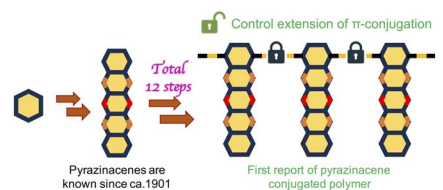
Christine S. Muli, Sergey G. Tarasov and Kylie J. Walters*



4054

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

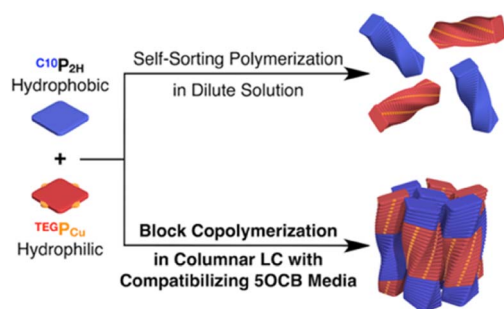
Fatima Hameed, Arindam Maity, Victor S. Francis and Nagarjuna Gavvalapalli*



- ✓ 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



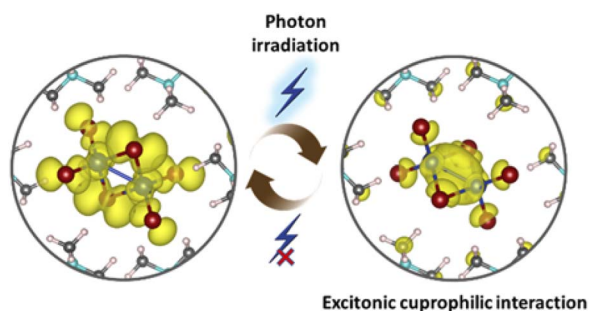
4068



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*

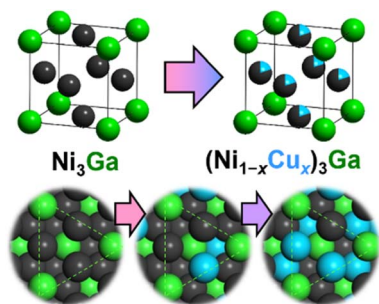
4075



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

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

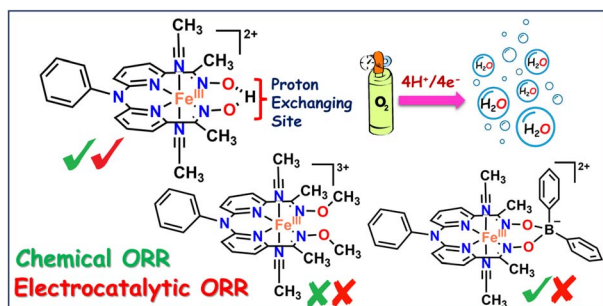
4086



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

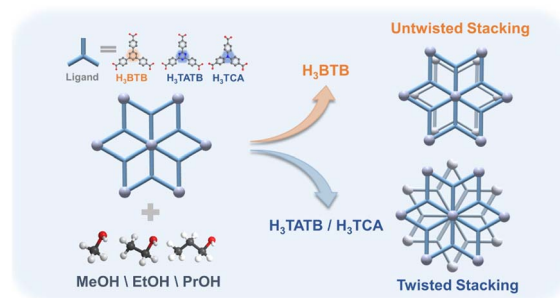
Aakash Santra, Avijit Das, Simarjeet Kaur, Priya Jain, Pravin P. Ingole and Sayantan Paria*



4106

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

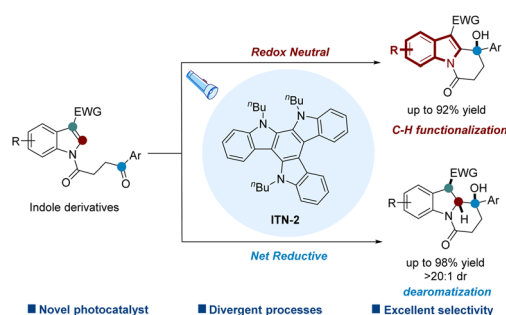
Yue Cheng, Wen-Qi Tang, Lu-Ting Geng, Ming Xu, Jian-Ping Zhu, Sha-Sha Meng and Zhi-Yuan Gu*



4114

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

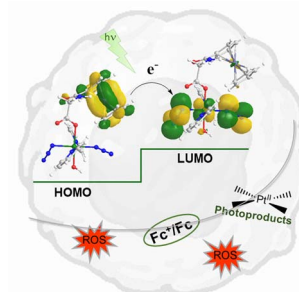
Bohang An, Hao Cui, Chao Zheng,* Ji-Lin Chen, Feng Lan, Shu-Li You* and Xiao Zhang*



4121

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

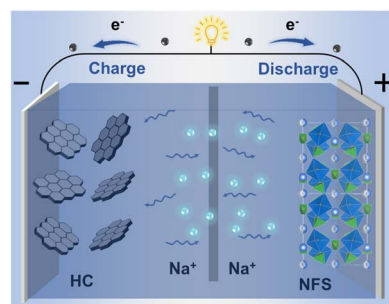
Huayun Shi, Fortuna Ponte, Jaspreet S. Grewal, Guy J. Clarkson, Cinzia Imberti, Ian Hands-Portman, Robert Dallmann, Emilia Sicilia* and Peter J. Sadler*



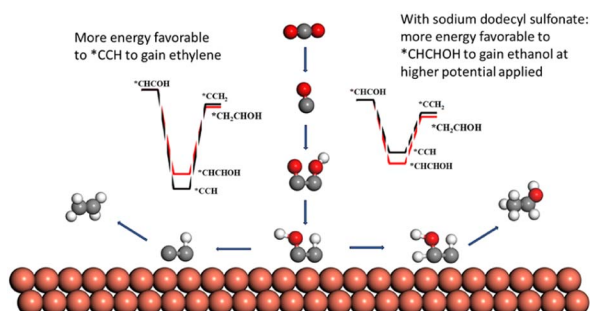
4135

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*



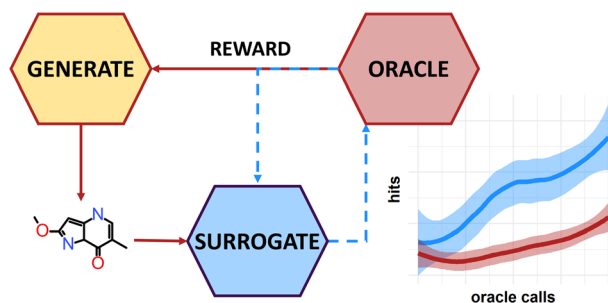
4140



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*

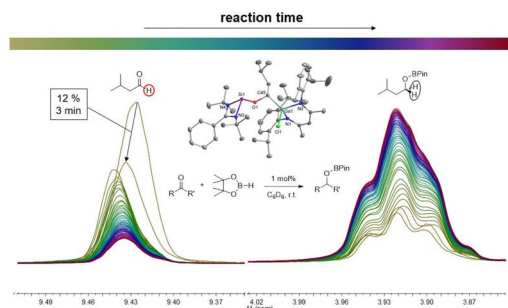
4146



Sample efficient reinforcement learning with active learning for molecular design

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

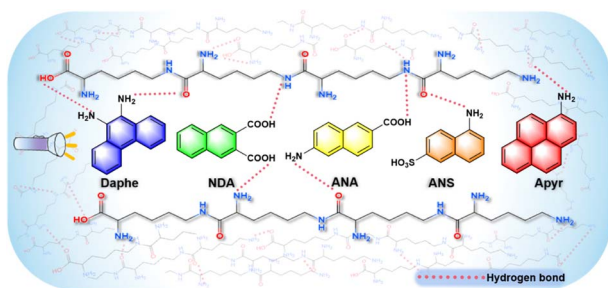
4161



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

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

4171



ϵ -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 $[(Cp^*Os)_2B_nH_n]$ ($n = 6-10$)

Ketaki Kar, Sourav Kar and Sundargopal Ghosh*

