

# Chemical Science

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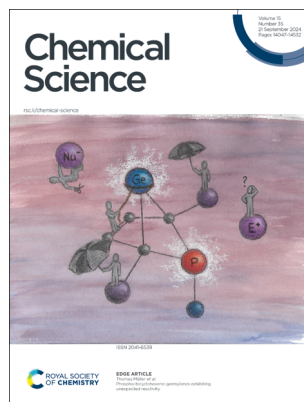
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## IN THIS ISSUE

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**Cover**  
See Lisa N. Kreimer and Terrance J. Hadlington, pp. 14154–14160. Image reproduced by permission of Terrance J. Hadlington from *Chem. Sci.*, 2024, 15, 14154.



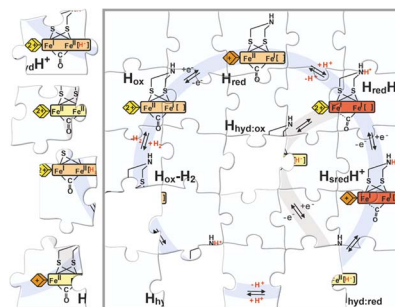
**Inside cover**  
See Thomas Müller *et al.*, pp. 14161–14170. Image reproduced by permission of Marie Sophie Würdemann from *Chem. Sci.*, 2024, 15, 14161.

## PERSPECTIVE

14062

### The missing pieces in the catalytic cycle of [FeFe] hydrogenases

Manon T. Lachmann, Zehui Duan, Patricia Rodríguez-Maciá\* and James A. Birrell\*

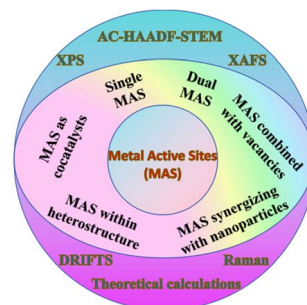


## REVIEWS

14081

### Recent advances of metal active sites in photocatalytic CO<sub>2</sub> reduction

Wa Gao,\* Haonan Li, Jianqiang Hu, Yong Yang,\* Yujie Xiong, Jinhua Ye, Zhigang Zou and Yong Zhou\*



# ChemComm

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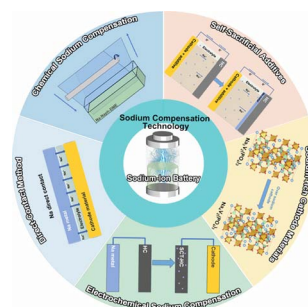
Fundamental questions  
Elemental answers

## REVIEWS

14104

## Sodium compensation: a critical technology for transforming batteries from sodium-starved to sodium-rich systems

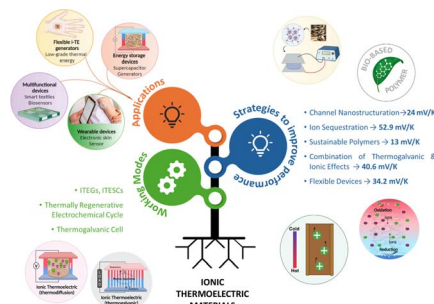
Bin Zhu, Wei Zhang,\* Zhenjing Jiang, Jie Chen, Zheng Li, Jingqiang Zheng, Naifeng Wen, Ruwei Chen, Hang Yang, Wei Zong, Yuhang Dai, Chumei Ye, Qi Zhang, Tianyun Qiu, Yanqing Lai, Jie Li and Zhian Zhang\*



14122

## Recent advances in ionic thermoelectric systems and theoretical modelling

Nazish Jabeen, Muhammad Muddasar, Nicolás Menéndez, Mohammad Ali Nasiri, Clara M. Gómez, Maurice N. Collins, Rafael Muñoz-Espí, Andrés Cantarero and Mario Culebras\*

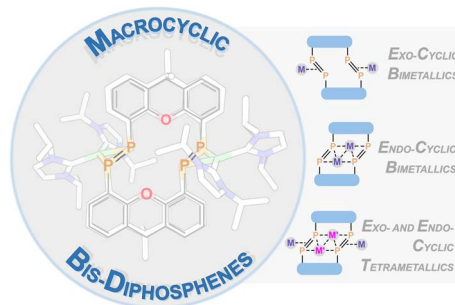


## EDGE ARTICLES

14154

## Macrocyclic bis-diphosphenes demonstrating bimetallic *exo*- and *endo*-cyclic binding modes

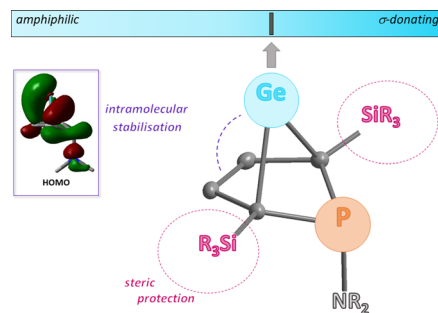
Lisa N. Kreimer and Terrance J. Hadlington\*



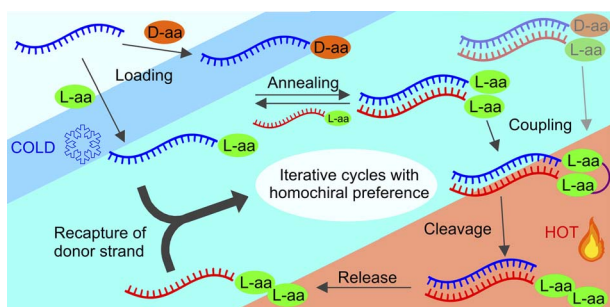
14161

## Phospha-bicyclohexene-germylenes exhibiting unexpected reactivity

Marie Sophie Würdemann, Steffen Kühn, Tobias Bötel, Marc Schmidtmann and Thomas Müller\*



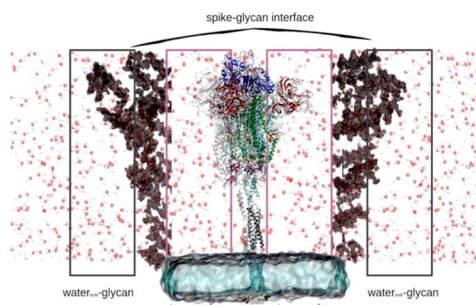
14171



### Gradual evolution of a homo-L-peptide world on homo-D-configured RNA and DNA

Ewa Węgrzyn, Ivana Mejdrová and Thomas Carell\*

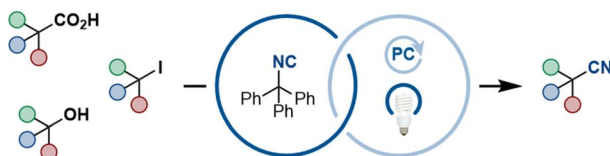
14177



### Water-glycan interactions drive the SARS-CoV-2 spike dynamics: insights into glycan-gate control and camouflage mechanisms

Marharyta Blazhynska, Louis Lagardère,\* Chengwen Liu, Olivier Adjoua, Pengyu Ren and Jean-Philip Piquemal\*

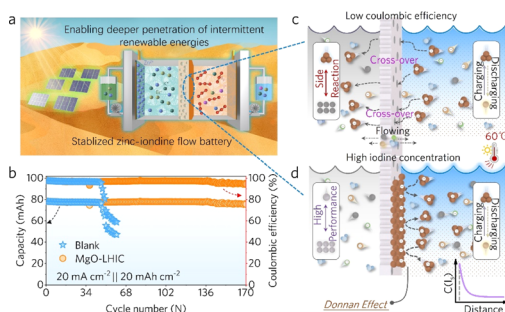
14188



### Trityl isocyanide as a general reagent for visible light mediated photoredox-catalyzed cyanations

Irene Quirós, María Martín, Carla Pérez-Sánchez, Thomas Rigotti\* and Mariola Tortosa\*

14195



### Initiating a composite membrane with a localized high iodine concentration layer based on adduct chemistry to enable highly reversible zinc-iodine flow batteries

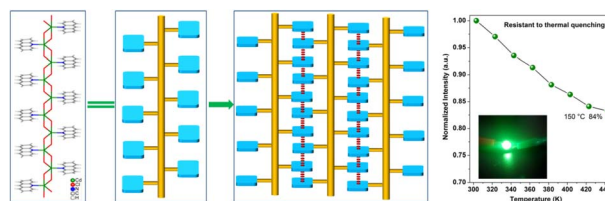
Yichan Hu, Tao Hu, Yuanwei Zhang, Haichao Huang, Yixian Pei, Yihan Yang, Yudong Wu, Haibo Hu,\* Guojin Liang\* and Hui-Ming Cheng



14202

### Low thermal quenching of metal halide-based metal–organic framework phosphor for light-emitting diodes

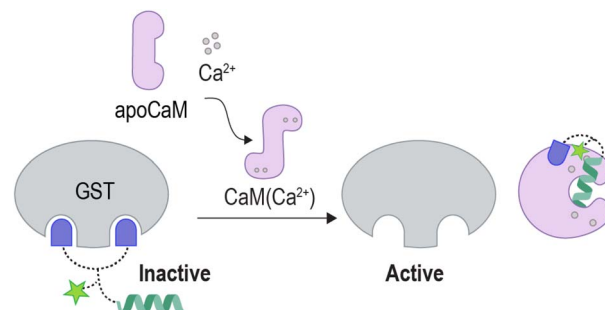
Xiao-Gang Yang,<sup>\*</sup> Ying-Jun Chen, Pei-Pei Yin, Yan Li, Shu-Yao Yang, Yi-Man Li and Lu-Fang Ma<sup>\*</sup>



14209

### Unnatural enzyme activation by a metal-responsive regulatory protein

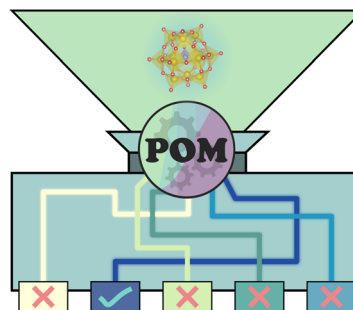
Olga Halfin, Liat Avram, Shira Albeck, Tamar Unger, Leila Motiei and David Margulies<sup>\*</sup>



14218

### Computational insights into aqueous speciation of metal-oxide nanoclusters: an in-depth study of the Keggin phosphomolybdate

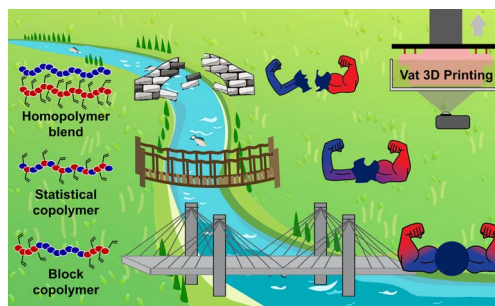
Jordi Buils, Diego Garay-Ruiz,<sup>\*</sup> Mireia Segado-Centellas, Enric Petrus and Carles Bo<sup>\*</sup>



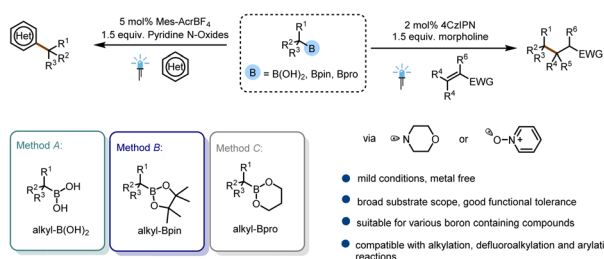
14228

### Bridging polymer architecture, printability, and properties by digital light processing of block copolycarbonates

Krista G. Schoonover, Chia-Min Hsieh, Mani Sengoden, Naushad Ahmed, Manivannan Sivaperuman Kalairaj, Taylor H. Ware, Donald J. Darensbourg,<sup>\*</sup> Emily B. Pentzer<sup>\*</sup> and Peiran Wei<sup>\*</sup>



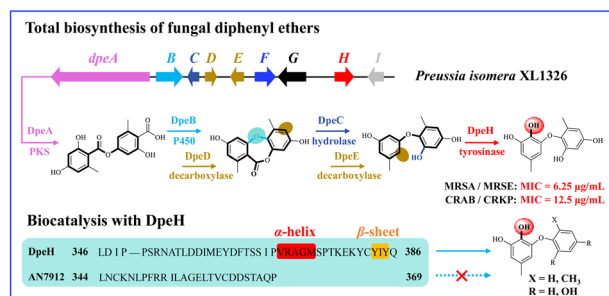
14241



## Deboronative functionalization of alkylboron species via a radical-transfer strategy

Fuyang Yue, Mingxing Li, Kangkang Yang, Hongjian Song, Yuxiu Liu and Qingmin Wang\*

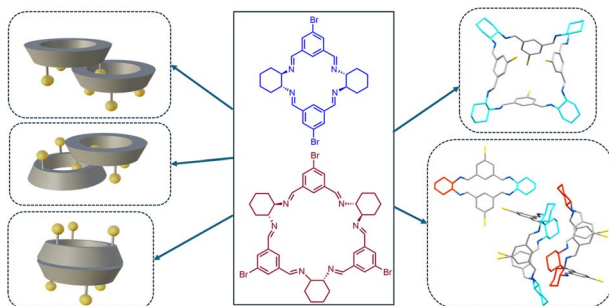
14248



## Novel fungal diphenyl ether biosynthetic gene clusters encode a promiscuous oxidase for elevated antibacterial activities

Qingpei Liu, Shuaibiao Gao, Jin Fang, Yifu Gong, Yiling Zheng, Yao Xu, Dan Zhang, Jiayuan Wei, Liangxiu Liao, Ming Yao, Wenjing Wang, Xiaole Han, Fusheng Chen, István Molnár\* and Xiaolong Yang\*

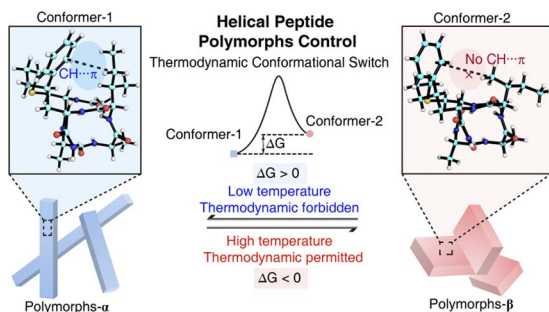
14254



## Dynamic and solid-state behaviour of bromoisotrianglimine

Abbie M. Scholes, Laurence J. Kershaw Cook, Filip T. Szczypiński, Konstantin V. Luzyanin, Benjamin D. Egleston, Rebecca L. Greenaway and Anna G. Slater\*

14264



## Intramolecular CH... $\pi$ attraction mediated conformational polymorphism of constrained helical peptides

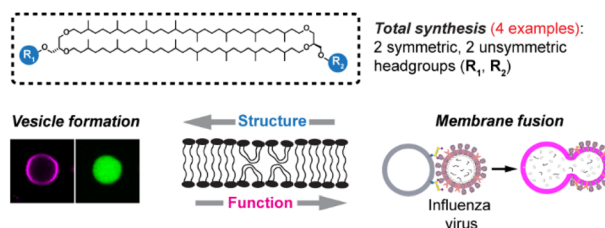
Jinming Sun, Zi-You Tian, Jianbo Liu, Chuan Wan, Chuan Dai, Zhihong Liu, Yun Xing, Yujie Wu, Zhanfeng Hou, Wei Han, Feng Yin,\* Yuxin Ye\* and Zigang Li\*



14273

### Structure–function relationships in pure archaeal bipolar tetraether lipids

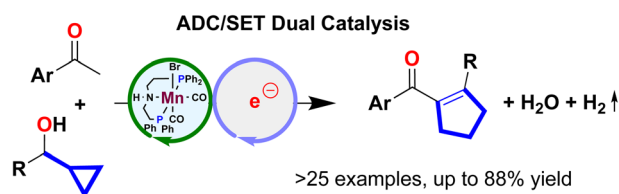
Ahanjit Bhattacharya, Isaac D. Falk, Frank R. Moss, III, Thomas M. Weiss, Khoi N. Tran, Noah Z. Burns\* and Steven G. Boxer\*



14287

### Manganese catalyzed chemo-selective synthesis of acyl cyclopentenes: a combined experimental and computational investigation

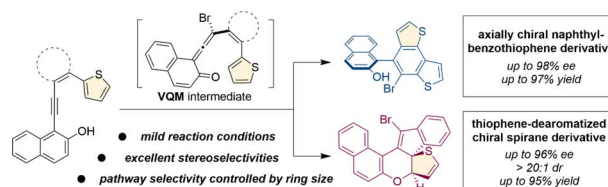
Koushik Sarkar, Prativa Behera, Lisa Roy\* and Biplab Maji\*



14295

### Catalytic asymmetric functionalization and dearomatization of thiophenes

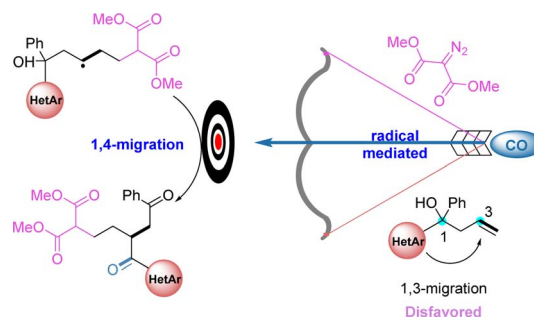
Zhengxing Zhao, Yingxin Li, Shiqi Jia,\* Lei Peng, Zian Zhang, Fengdi Wu, Pengfei Wang, Wenling Qin,\* Yu Lan and Hailong Yan\*



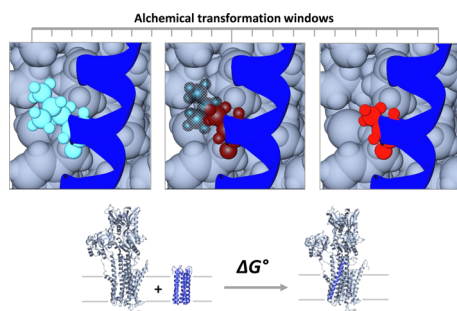
14304

### Visible light induced cooperative carbonylation and (hetero)aryl migration: synthesis of multi-carbonyl compounds

Hefei Yang, Yuanrui Wang, Le-Cheng Wang and Xiao-Feng Wu\*



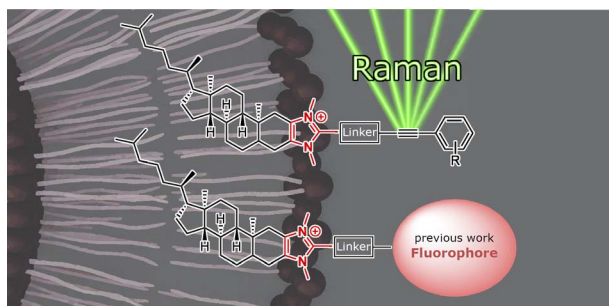
14310



### Probing the formation of a hetero-dimeric membrane transport complex with dual *in vitro* and *in silico* mutagenesis

Nishadh Rathod, M. Joanne Lemieux, Christophe Chipot, Benoît Roux and Howard S. Young\*

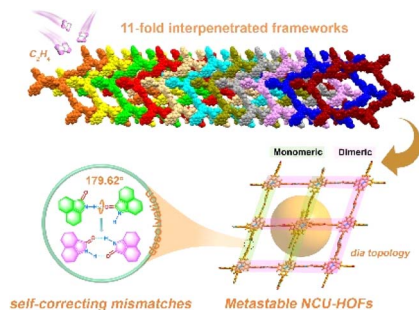
14323



### Alkyne-tagged imidazolium-based membrane cholesterol analogs for Raman imaging applications

Constanze Schultz, Tristan Wegner, Corinna Heusel, Tim Gallagher, Yanjun Zheng, Markus Werner, Seraphine V. Wegner, Tobias Meyer-Zedler, Oliver Werz, Michael Schmitt, Juergen Popp\* and Frank Glorius\*

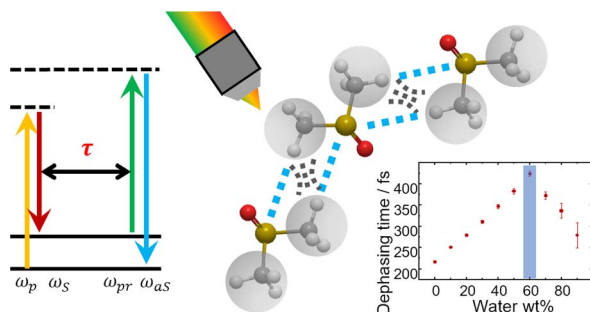
14336



### Self-correcting mismatches in metastable hydrogen-bonded organic frameworks with an 11-fold interpenetrated array

Guomin Xia, Chunlei Zhou, Xingliang Xiao, Yang Yang, Fuqing Yu and Hongming Wang\*

14344



### Dynamics of CH/*n* hydrogen bond networks probed by time-resolved CARS spectroscopy

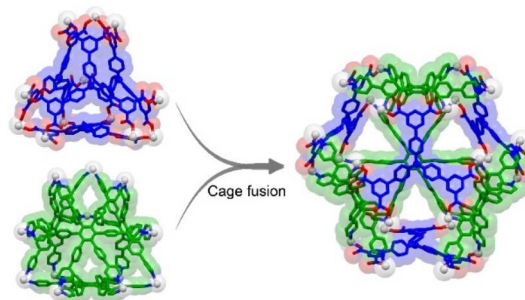
Hanlin Zhu, Xinyu Deng, Vladislav V. Yakovlev\* and Delong Zhang\*



14352

### Fusion of two homoleptic truncated tetrahedra into a heteroleptic truncated octahedron

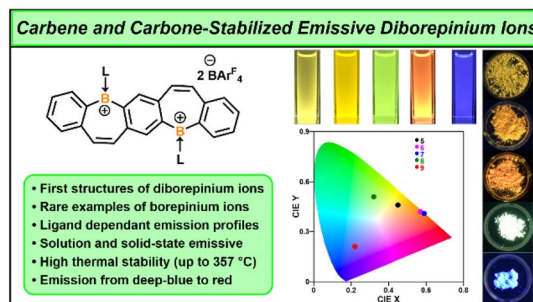
Haifei Liu, Chenxing Guo, Yujuan Huang, Zilin Zhou, Shijin Jian, Zeyuan Zhang, Yali Hou, Chaoqun Mu\* and Mingming Zhang\*



14358

### Pentacyclic fused diborepinium ions with carbene- and carbene-mediated deep-blue to red emission

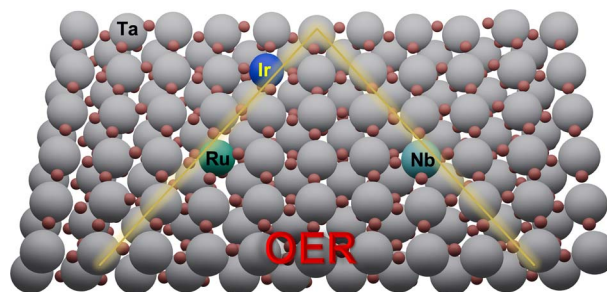
Kimberly K. Hollister, Andrew Molino, VuongVy V. Le, Nula Jones, Wyatt J. Smith, Peter Müller, Diane A. Dickie, David J. D. Wilson\* and Robert J. Gilliard, Jr\*



14371

### Understanding the catalytic performances of metal-doped Ta<sub>2</sub>O<sub>5</sub> catalysts for acidic oxygen evolution reaction with computations

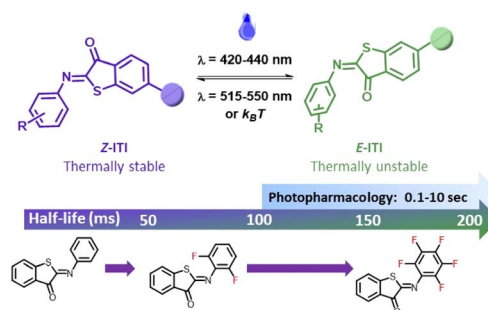
Congcong Han and Tao Wang\*



14379

### Getting a molecular grip on the half-lives of iminothioindoxyl photoswitches

Melody E. Boëtius, Mark W. H. Hoorens, Martin Oštdnický, Adèle D. Laurent, Mariangela di Donato, Aldo C. A. van Wingarden, Michiel F. Hilbers, Ben L. Feringa, Wybren Jan Buma,\* Miroslav MedvedĚ\* and Wiktor Szymanski\*



14390

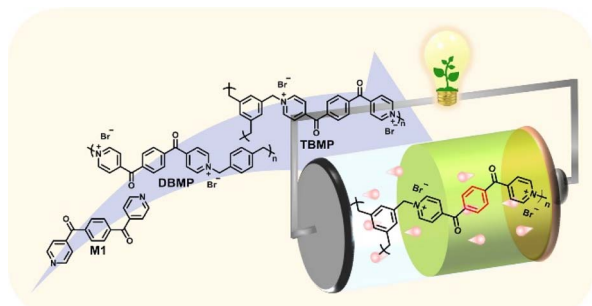
## Organometallic Spin Qubits



### ( $\eta^8$ -Cyclooctatetraene)( $\eta^5$ -fluorenyl)titanium: a processable molecular spin qubit with optimized control of the molecule–substrate interface

Sarita Wisbeck, Andrea Luigi Sorrentino, Francielli S. Santana, Luana C. de Camargo, Ronny R. Ribeiro, Enrico Salvadori, Mario Chiesa, Niccolò Giaconi, Andrea Caneschi, Matteo Mannini, Lorenzo Poggini, Matteo Briganti,\* Giulia Serrano,\* Jaísa F. Soares\* and Roberta Sessoli\*

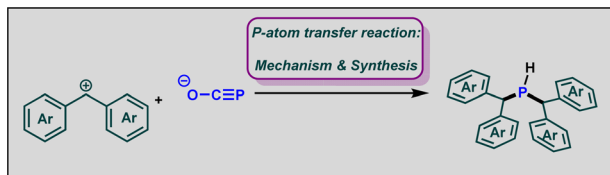
14399



### Cross-linking enhances the performance of four-electron carbonylpyridinium based polymers for lithium organic batteries

Hongyan Li, Ling Chen, Fangfang Xing, Hongya Miao, Jing Zeng, Sen Zhang and Xiaoming He\*

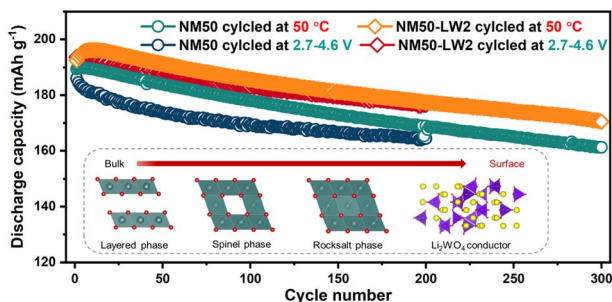
14406



### Reactivity of the phosphathynolate anion with stabilized carbocations: mechanistic studies and synthetic applications

Thi Hong Van Nguyen, Saloua Chelli, Sonia Mallet-Ladeira, Martin Breugst\* and Sami Lakhdar\*

14415



### Slightly Li-enriched chemistry enabling super stable LiNi<sub>0.5</sub>Mn<sub>0.5</sub>O<sub>2</sub> cathodes under extreme conditions

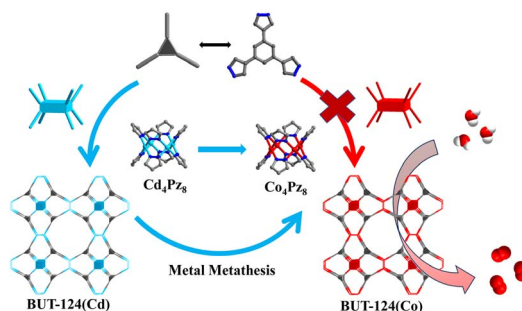
Siqi Chen, Ping Zhang, Xin Zhou, Wenbin Wu, Xiaohong Liu,\* Yifeng Liu, Guilin Feng, Bin Zhang, Wangyan Xing, Meihua Zuo, Ping Zhang, Genpin Lv, Yao Xiao,\* Shixue Dou and Wei Xiang\*



14425

### Unlocking the potential: strategic synthesis of a previously predicted pyrazolate-based stable MOF with unique clusters and high catalytic activity

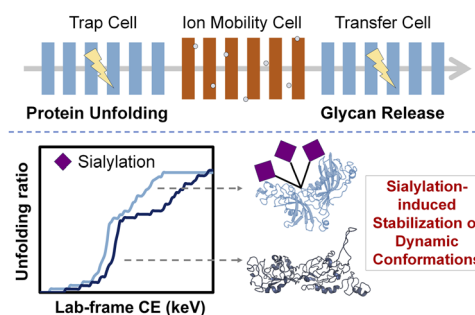
Xiang-Yu Li, Yan-Long Zhao, Su-Nan Chen, Kecheng Wang,\* Shengjun Wang, Lin-Hua Xie\* and Jian-Rong Li\*



14431

### Sialylation-induced stabilization of dynamic glycoprotein conformations unveiled by time-aligned parallel unfolding and glycan release mass spectrometry

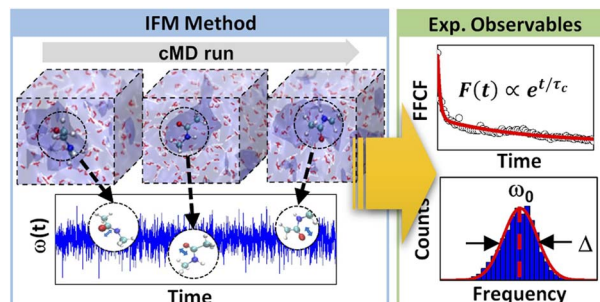
Yifei Jia, Yichang Liu, Yamei Wang, Jinyu Li\* and Gongyu Li\*



14440

### A new computational methodology for the characterization of complex molecular environments using IR spectroscopy: bridging the gap between experiments and computations

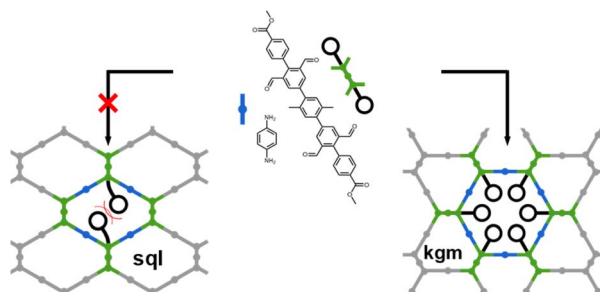
Laura X. Sepulveda-Montaño, Johan F. Galindo and Daniel G. Kuroda\*



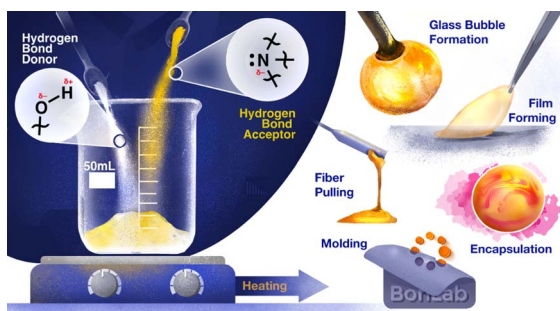
14449

### Enhancing structural control in covalent organic frameworks through steric interaction-driven linker design

Alena Winter, Farzad Hamdi, Andreas Eichhöfer, Kay Saalwächter, Panagiotis L. Kastiris and Frederik Haase\*



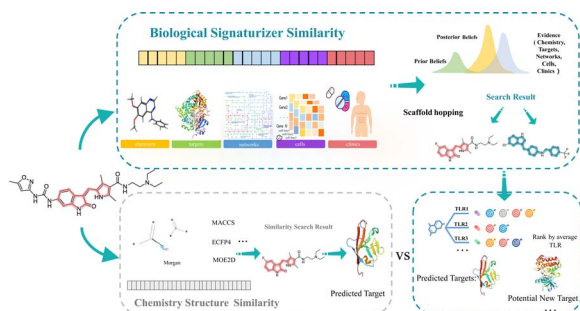
14458



### Small molecule organic eutectics as candidates to replace plastics

Joshua L. Ryan, Gabriele C. Sosso\* and Stefan A. F. Bon\*

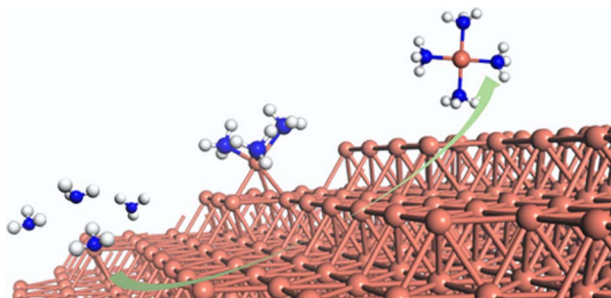
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### Predicting novel targets with Bayesian machine learning by integrating multiple biological signatures

Xiao Wei, Tingfei Zhu, Hiu Fung Yip, Xiangzheng Fu, Dejun Jiang, Youchao Deng, Aiping Lu and Dongsheng Cao\*

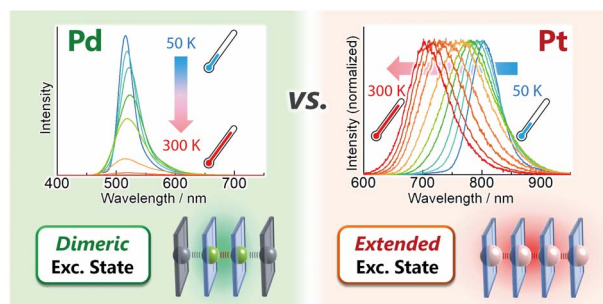
14485



### Origin of copper dissolution under electrocatalytic reduction conditions involving amines

Yani Guan, Justus Kümper, Sonja D. Mürtz, Simran Kumari, Peter J. C. Hausoul, Regina Palkovits\* and Philippe Sautet\*

14497



### Thermo-responsive emission induced by different delocalized excited-states in isomorphous Pd(II) and Pt(II) one-dimensional chains

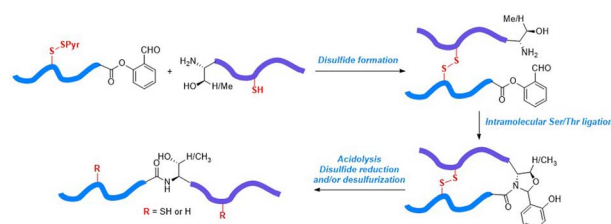
Tomoya Saito, Masaki Yoshida,\* Kaito Segawa, Daisuke Saito, Junichi Takayama, Satoshi Hiura, Akihiro Murayama, Nishshanka M. Lakshan, W. M. C. Sameera, Atsushi Kobayashi and Masako Kato\*



14506

**Prior disulfide bond-mediated Ser/Thr ligation**

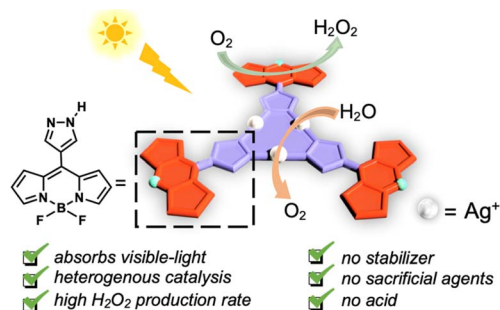
Heng Liu, Hoi Yee Chow, Jiamei Liu, Pengfei Shi and Xuechen Li\*



14513

**A cyclic trinuclear silver complex for photosynthesis of hydrogen peroxide**

Ri-Qin Xia, Zhen-Na Liu, Yu-Ying Tang, Xiao Luo, Rong-Jia Wei, Tao Wu, Guo-Hong Ning\* and Dan Li\*



14521

**Surface topology of MXene flakes induces the selection of the sintering mechanism for supported Pt nanoparticles**

Jiawei Huang, Yucheng Zhang, Jiaqi Chen, Zhouyang Zhang, Chunfang Zhang,\* Changshui Huang\* and Linfeng Fei\*

