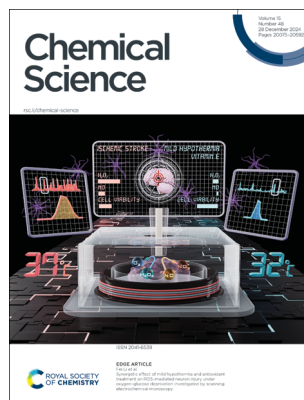


## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(48) 20075–20592 (2024)



**Cover**  
See Zihao Guo, Jieping Wang, Wenbin Yi *et al.*, pp. 20171–20176. Image reproduced by permission of Wenbin Yi from *Chem. Sci.*, 2024, 15, 20171.



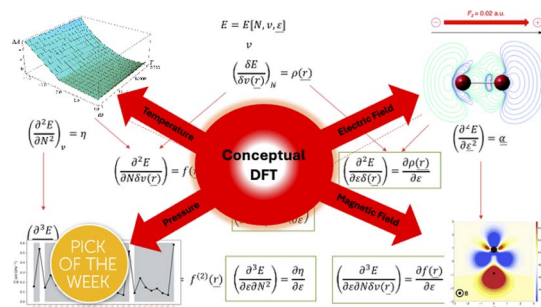
**Inside cover**  
See Fei Li *et al.*, pp. 20177–20188. Image reproduced by permission of Fei Li from *Chem. Sci.*, 2024, 15, 20177. Artwork by Chengjun Zhao.

## PERSPECTIVES

20090

### Temperature and external fields in conceptual density functional theory

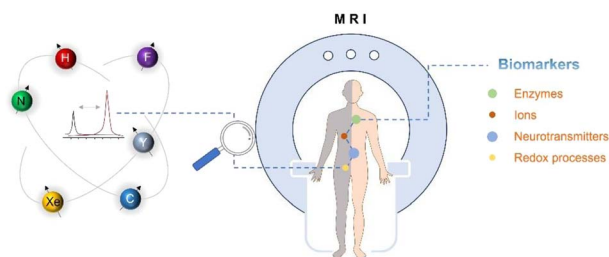
Marco Franco-Pérez,\* Farnaz Heidar-Zadeh,\* Paul W. Ayers,\* Frank De Proft,\* Alberto Vela,\* José L. Gázquez\* and Paul Geerlings\*



20122

### The role of responsive MRI probes in the past and the future of molecular imaging

Ping Yue, Thavasilingham Nagendraraj, Gaoji Wang, Ziyi Jin and Goran Angelovski\*



# Environmental Science: Atmospheres

GOLD  
OPEN  
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Connecting communities  
and inspiring new ideas

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Fundamental questions  
Elemental answers

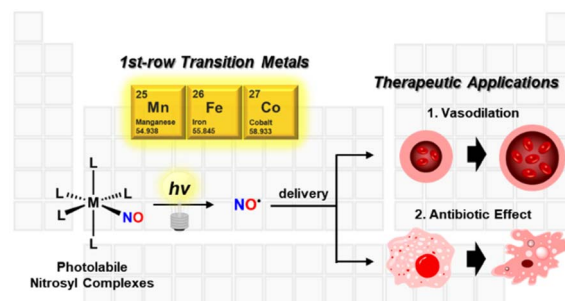


## REVIEW

20155

## Photo-triggered NO release of nitrosyl complexes bearing first-row transition metals and therapeutic applications

Seungwon Sun, Jisu Choe and Jaeheung Cho\*

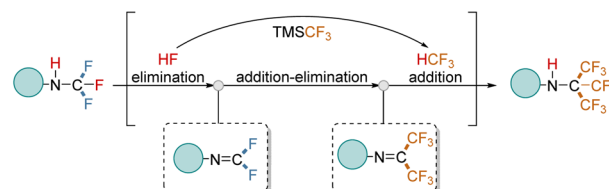


## EDGE ARTICLES

20171

## Direct synthesis of *N*-perfluoro-*tert*-butyl secondary amines from *N*-trifluoromethyl secondary amines

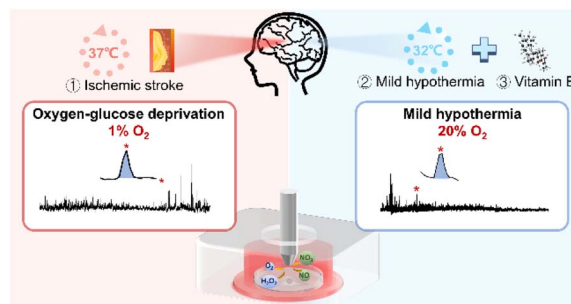
Leibing Wang, Zhongyu Feng, Zhen Luo, Zihao Guo,\* Jieping Wang\* and Wenbin Yi\*



20177

## Synergetic effect of mild hypothermia and antioxidant treatment on ROS-mediated neuron injury under oxygen-glucose deprivation investigated by scanning electrochemical microscopy

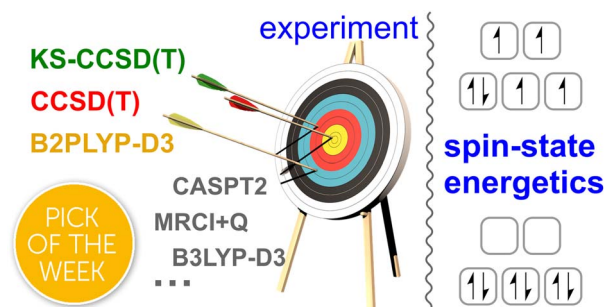
Junjie Zhang, Yulin Liu, Yuxiang Zhao, Siyu Zhang, Feng Xu and Fei Li\*



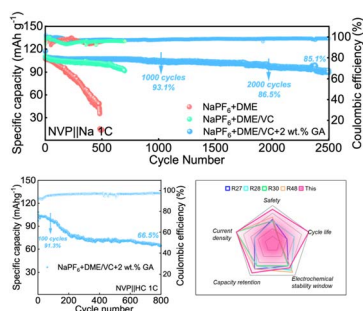
20189

## Performance of quantum chemistry methods for a benchmark set of spin-state energetics derived from experimental data of 17 transition metal complexes (SSE17)

Mariusz Radoń,\* Gabriela Drabik, Maciej Hodorowicz and Janusz Szklarzewicz



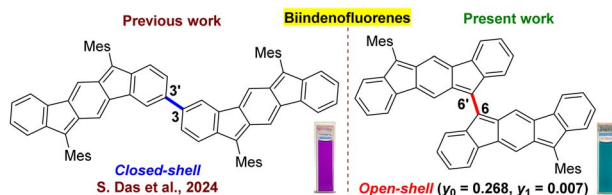
20205



### Ultra-long cycle sodium ion batteries enabled by the glutaric anhydride additive

Qin Zhou, Cong Xia, Zhifan Kuang, Mengran Guo, Hao Zhang, Haojie Wan, Shiquan Wang,<sup>\*</sup> Lin Li<sup>\*</sup> and Jianwen Liu<sup>\*</sup>

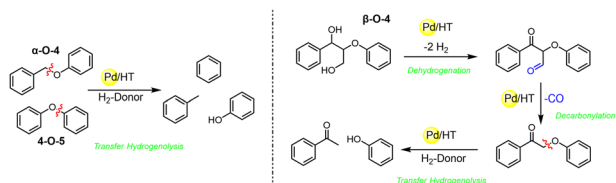
20215



### 6,6'-Biindenofluorene: an open-shell indenofluorene dimer

Himanshu Sharma, Palash Jana, Dibyendu Mallick, Subhajit Bandyopadhyay and Soumyajit Das<sup>\*</sup>

20223



### Selective lignin depolymerization via transfer hydrogenolysis using Pd/hydrotaicite catalysts: model compounds to whole biomass

Darren Dolan, Rebekah Brucato, Christopher Reid, Adam F. Lee,<sup>\*</sup> Karen Wilson<sup>\*</sup> and Adelina M. Voutchkova-Kostal<sup>\*</sup>

20240



### Enhanced efficiency in plastic waste upcycling: the role of mesoporosity and acidity in zeolites

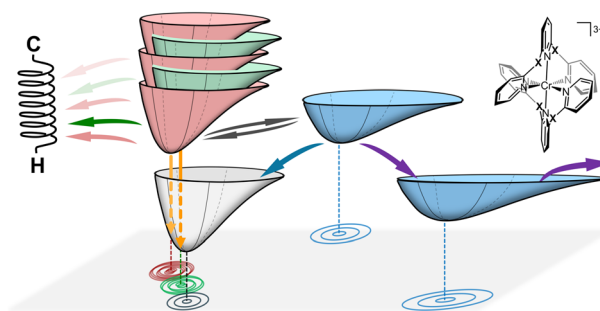
Saideep Singh, Joaquín Martínez-Ortigosa, Nuria Ortuño, Vivek Polshettiwar<sup>\*</sup> and Javier García-Martínez<sup>\*</sup>



20251

### Bridge editing of spin-flip emitters gives insight into excited state energies and dynamics

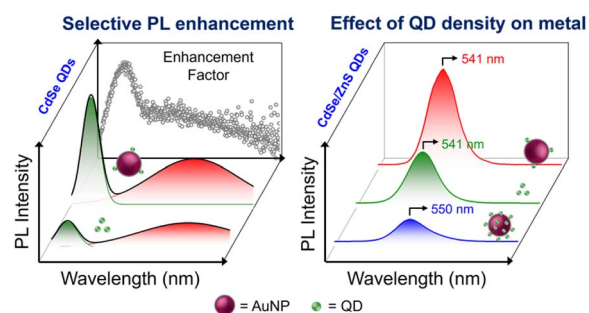
Florian Reichenauer, Robert Naumann, Christoph Förster, Winald R. Kitzmann, Antti-Pekka M. Reponen, Sascha Feldmann and Katja Heinze\*



20263

### Resonance plasmonic coupling: selective enhancement of band edge emission over trap state emission of CdSe quantum dots

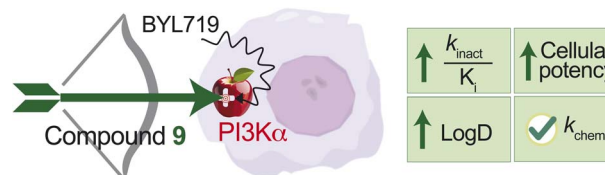
Livin Paul, Elizabeth Mariam Thomas, Akshaya Chemmangat, Stephen K. Gray\* and K. George Thomas\*



20274

### Rapid, potent, and persistent covalent chemical probes to deconvolute PI3K $\alpha$ signaling

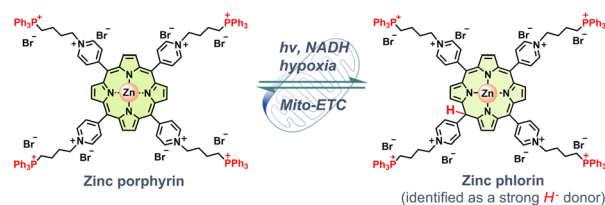
Lukas Bissegger, Theodora A. Constantin, Erhan Keles, Luka Raguž, Isobel Barlow-Busch, Clara Orbeago, Thorsten Schaefer, Valentina Borlandelli, Thomas Bohnacker, Rohitha Sriramaratnam, Alexander Schäfer, Matthias Gstaiger, John E. Burke, Chiara Borsari and Matthias P. Wymann\*



20292

### Photoactivated hydride therapy under hypoxia beyond ROS

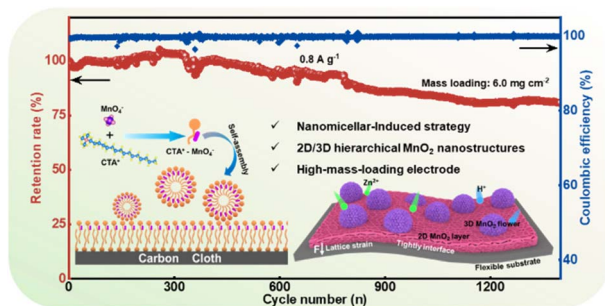
Xia Wang, Yijian Gao, Ting Wang, Zhaobin Wang, He Hang, Shengliang Li\* and Fude Feng\*



- ✓ Target Mito-ETC via  $H^-$  transfer
- ✓ Mitochondrial NADH as a cancer biomarker
- ✓ Hypoxia-tolerant & ROS-independent
- ✓ Spare normal and macrophage cells



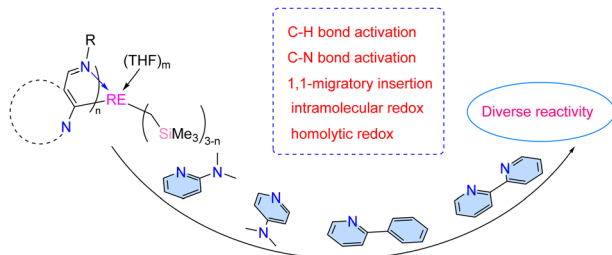
20303



### Tailoring hierarchical MnO<sub>2</sub> nanostructures on self-supporting cathodes for high-mass-loading zinc-ion batteries

Weijie Zheng, Zhibiao Cui, Cong Liu, Libei Yuan, Shengsong Li, Lilin Lin, Tao Meng,\* Liangui Yang, Yexiang Tong and Dong Shu\*

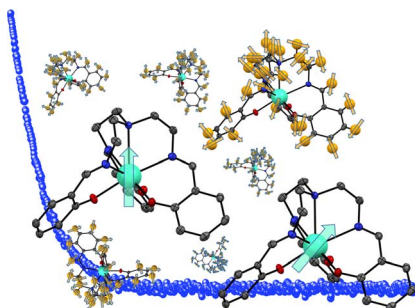
20315



### Rare-earth metal complexes bearing electrophilic and nucleophilic carbon centres and their unique reactivity patterns towards pyridine derivatives

Weikang Wu, Thayalan Rajeshkumar, Shan Zhu, Fuxiang Chai, Dongjing Hong, Zeming Huang, Qingbing Yuan, Laurent Maron\* and Shaowu Wang\*

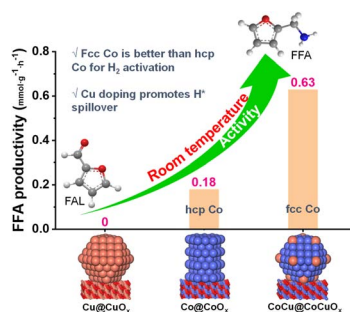
20328



### Probing decoherence in molecular 4f qubits

Steen H. Hansen, Christian D. Buch, Jonatan B. Petersen, Michelle Rix, Marc Ubach I Cervera, Asger Strandfelt, Richard E. P. Winpenny, Eric J. L. McInnes and Stergios Piligkos\*

20338



### Phase transition induced hydrogen activation for enhanced furfural reductive amination over a CoCu bimetallic catalyst

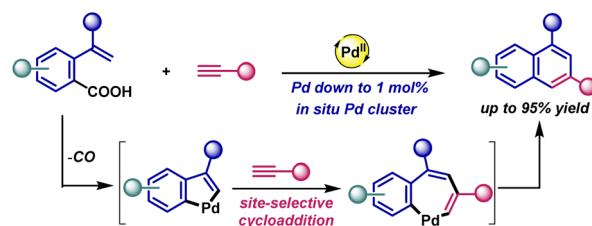
Yilin Wei, Zixu Ma, Beibei Liu, Jialin Yang, Dan Wu, Yongsheng Zhang, Yuexing Zhang,\* Chunbao Charles Xu and Renfeng Nie\*



20346

### Site-selective decarbonylative [4 + 2] annulation of carboxylic acids with terminal alkynes by C–C/C–H activation strategy and cluster catalysis

Mengjie Cen, Xinyue Ma, Xi Yang, Shangshang Zhang, Long Liu, Michal Szostak\* and Tieqiao Chen\*

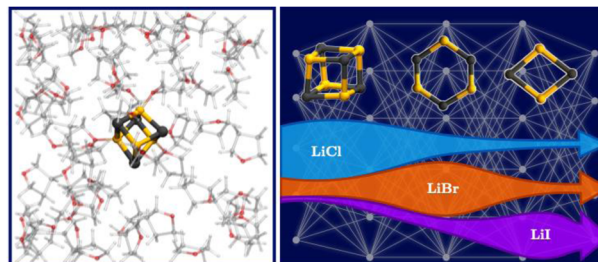


- Decarbonylative cyclization forming naphthalenes
- High regio-selectivity
- Readily available starting materials
- High functional group tolerance
- Synthesis of molecules with bioactive complex fragments
- Scalable

20355

### Morphology of lithium halides in tetrahydrofuran from molecular dynamics with machine learning potentials

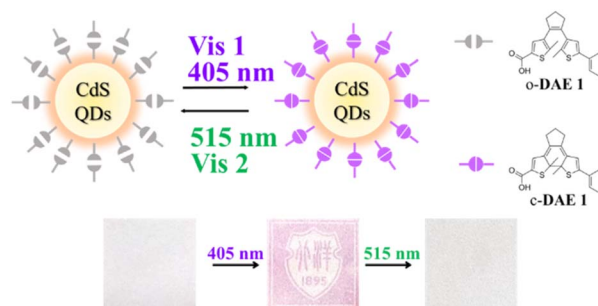
Marinella de Giovanetti, Sondre Hilmar Hopen Eliasson, Sigbjørn Løland Bore, Odile Eisenstein\* and Michele Cascella\*



20365

### An efficient all-visible light-activated photoswitch based on diarylethenes and CdS quantum dots

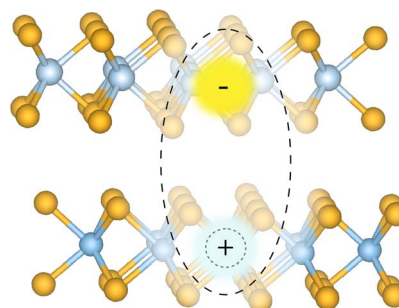
Kezhou Chen, Jiayi Liu, Joakim Andréasson, Bo Albinsson,\* Tiegen Liu\* and Lili Hou\*



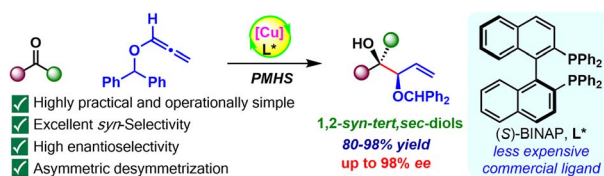
20371

### Molecular origins of exciton condensation in van der Waals heterostructure bilayers

Lillian I. Payne Torres, Anna O. Schouten and David A. Mazziotti\*



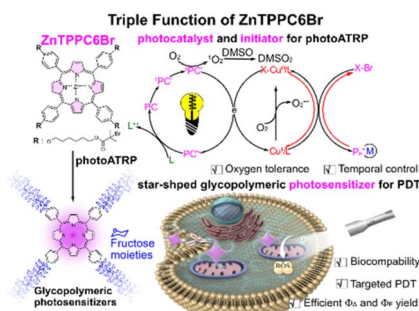
20379



### BINAP-CuH-catalysed enantioselective allylation using alkoxyallenes to access 1,2-*syn-tert,sec*-diols

N. Navaneetha, Sundaram Maurya, Prativa Behera, Sandip B. Jadhav, Lakshmi Revati Magham, Jagadeesh Babu Nanubolu, Lisa Roy\* and Rambabu Chegondi\*

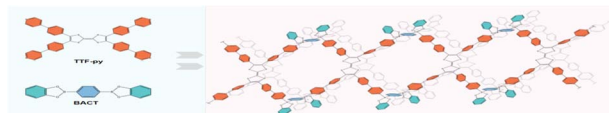
20388



### Triple-function porphyrin in glycopolymeric photosensitizers: from photoATRP to targeted PDT

Jiahui Lin, Zhiyuan Ma,\* Weiwei Zuo and Meifang Zhu

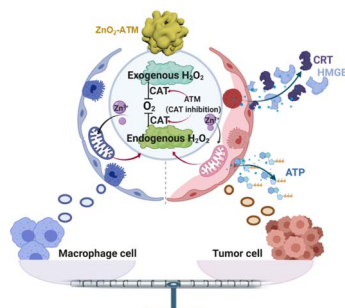
20397



### A tetrathiafulvalene-containing covalent organic nanobelt: preparation, crystal structure and application for sodium-ion batteries

Xin Wang, Yuchan Zhang, Lei Zhang, Qianfeng Gu, Qi Liu, Yang Ren, Chun Sin Lee and Qichun Zhang\*

20403



### Bimodal accurate H<sub>2</sub>O<sub>2</sub> regulation to equalize tumor-associated macrophage repolarization and immunogenic tumor cell death elicitation

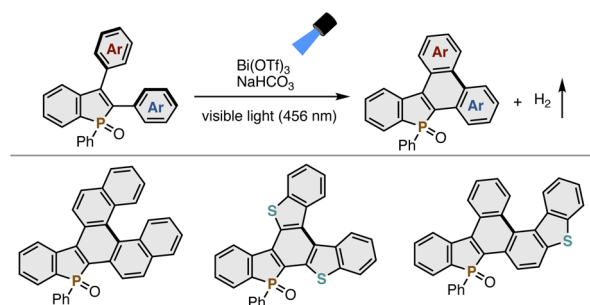
Yan Zhao, Weiheng Kong, Jianqing Zhu and Fengli Qu\*



20413

### Synthesis of highly condensed phospholes by the Lewis acid-assisted dehydrogenative Mallory reaction under visible light irradiation

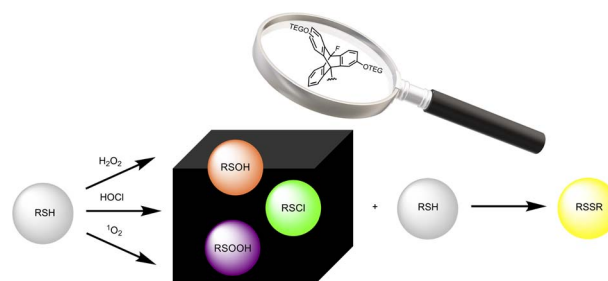
Ikki Kamiyoshi, Yuki Kojima, Shibo Xu, Kosuke Yasui, Yuji Nishii and Koji Hirano\*



20421

### Monitoring electrophilic intermediates in reactions of thiols in aqueous solution directly with $^{19}\text{F}$ NMR

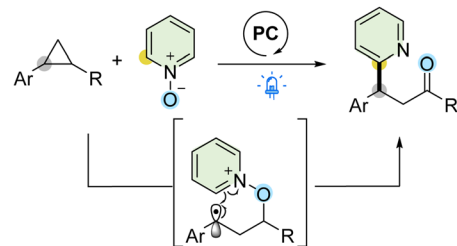
Dmitry D. Saraev and Derek A. Pratt\*



20433

### Photocatalytic 1,3-oxyheteroarylation of aryl cyclopropanes with azine *N*-oxides

Doyoung Kim, Hyewon Ju, Wooseok Lee and Sungwoo Hong\*

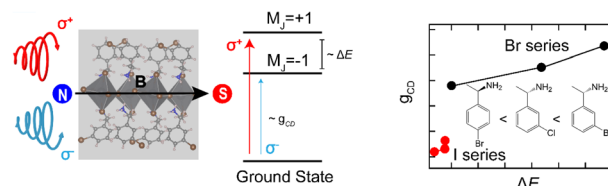


- broad aryl cyclopropanes
- transition metal-free
- *ortho*-selective pyridylation
- bifunctional reagent

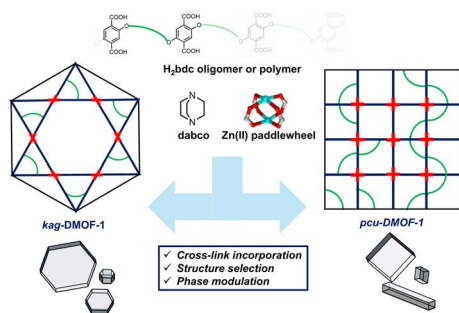
20440

### Deciphering the electronic and structural origin of chiroptical activity of chiral 2D perovskites

Zixuan Zhang, Jin Wu and Haipeng Lu\*



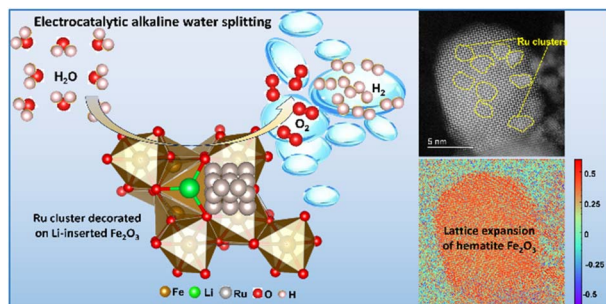
20448



## Ligand cross-links as a design element in oligo- and polyMOFs

Debobroto Sensharma and Seth M. Cohen\*

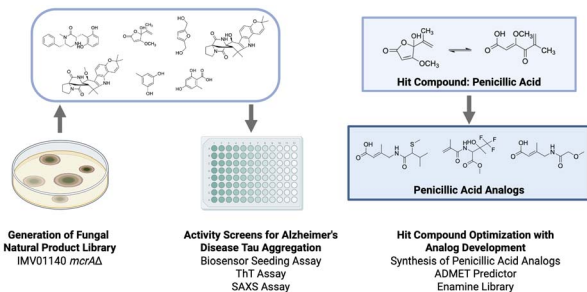
20457



## Ruthenium clusters decorated on lattice expanded hematite $\text{Fe}_2\text{O}_3$ for efficient electrocatalytic alkaline water splitting

Haibin Ma, Yongqiang Yang, Xiaohua Yu, Yang Zhao, Jiwei Ma\* and Hongfei Cheng\*

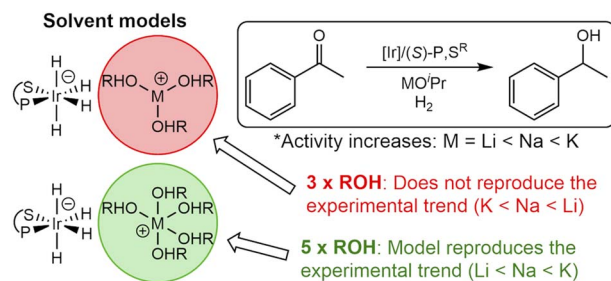
20467



## Discovery of penicillic acid as a chemical probe against tau aggregation in Alzheimer's disease

Jennifer Shyong, Jinliang Wang, Quoc-Dung Tran Huynh, Marina Fayzullina, Bo Yuan, Ching-Kuo Lee, Thomas Minehan, Paul M. Seidler\* and Clay C. C. Wang\*

20478



## Understanding ketone hydrogenation catalysis with anionic iridium(III) complexes: the crucial role of counterion and solvation

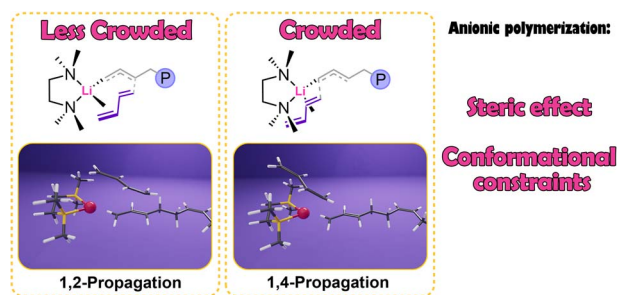
Paven Kisten, Sandrine Vincendeau, Eric Manoury, Jason M. Lynam, John M. Slattery,\* Simon B. Duckett, Agustí Lledós\* and Rinaldo Poli\*



20493

### Unlocking regioselectivity: steric effects and conformational constraints of Lewis bases in alkyllithium-initiated butadiene polymerization

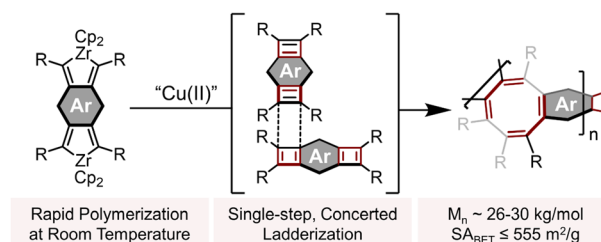
Jian Tang, Yuan Fu, Jing Hua,\* Jiahao Zhang, Shuoli Peng and Zhibo Li



20503

### Direct ladderization of cyclooctatetraene-containing, processable conjugated ladder polymers from annulated bis-zirconacyclopentadienes

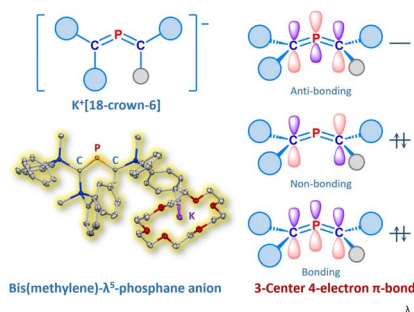
August J. Rothenberger, Harrison M. Bergman, He Li, Miao Qi, Yunfei Wang, Yi Liu\* and T. Don Tilley\*



20509

### Bis(methylene)- $\lambda^5$ -phosphane anions

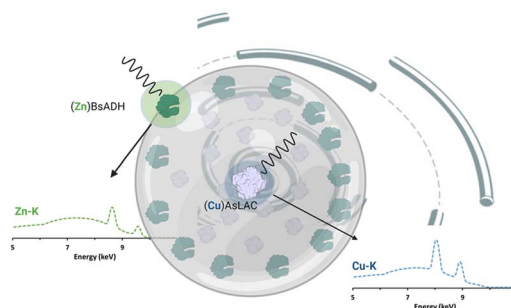
Akihiro Nomoto, Koh Sugamata\* and Takahiro Sasamori\*



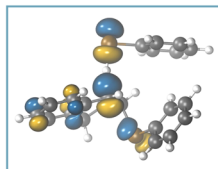
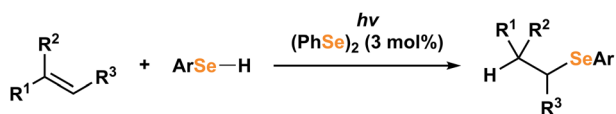
20515

### Unveiling the spatial rearrangements of exhausted immobilised multi-enzyme systems through cryo-X-ray fluorescence nanoprobe imaging

Javier Santiago-Arcos, Murielle Salome, Fernando López-Gallego\* and Carlos Sanchez-Cano\*



20523

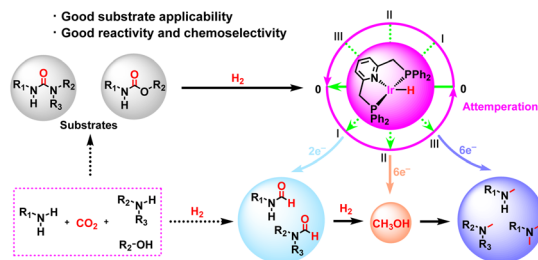


- high *anti*-selectivity •
- broad substrate scope •
- identification of  $\beta$ -selenide effect •

### Hydroselemination of olefins: elucidating the $\beta$ -selenium effect

Gabriel S. Phun, Hannah S. Slocumb, Kirsten J. Ruud, Shaozhen Nie, Cheyenne Antonio, Filipp Furche,\* Vy M. Dong\* and Xiao-Hui Yang\*

20534



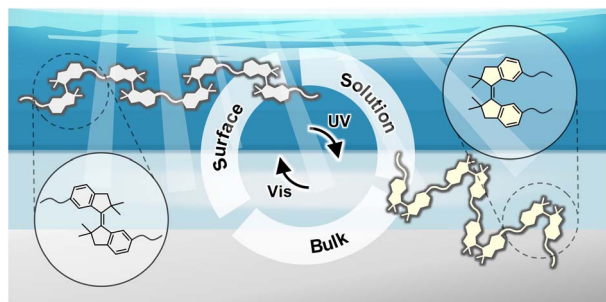
- Good substrate applicability
- Good reactivity and chemoselectivity

- Controllable production of multiple reduction products
- No external additives are required in this catalyst system

### Highly selective customized reduction products for hydrogenation of CO<sub>2</sub>-derived urea derivatives or carbamates

Jun Zhu, Yongtao Wang, Jia Yao and Haoran Li\*

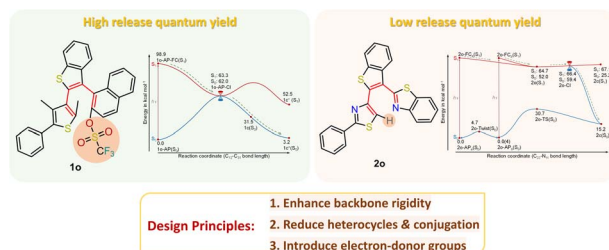
20545



### Main-chain stiff-stilbene photoswitches in solution, in bulk, and at surfaces

Naoki Kaneda, Keiichi Imato,\* Ayane Sasaki, Ryo Tanaka, Ichiro Imae, Toyooki Hirata, Takuya Matsumoto and Yousuke Ooyama\*

20556



### Exploring the molecular design principles for efficient diarylethene photoacid and photohydride generators based on the photochemical reaction mechanism

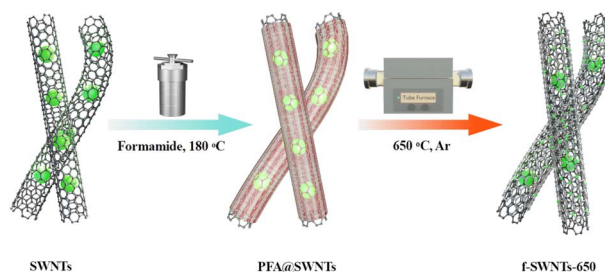
Yifan Su, Dexin Zheng, Lingfeng Ge, Le Yu,\* David Lee Phillips, Jiani Ma\* and Yu Fang



20565

### Partial thermal atomization of residual Ni NPs in single-walled carbon nanotubes for efficient CO<sub>2</sub> electroreduction

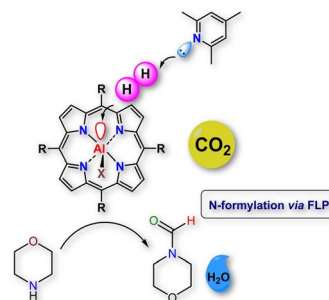
Fengwei Zhang,\* Han Zhang, Yang Zhao, Jingjing Li, Chong Guan, Jijie Li, Xuran Wang, Yuewen Mu, Wen-Yan Zan\* and Sheng Zhu\*



20573

### Aluminium porphyrins catalyse the hydrogenation of CO<sub>2</sub> with H<sub>2</sub>

Nitin Kumar, Gabriela Gastelu, Martin Zábanský, Jaroslav Kukla, Jorge G. Uranga\* and Martin Hulla\*



20582

### Reactivity of metal hydrides with CO<sub>2</sub>: going beyond formate with a high-valent cationic pentahydride Mo(vi) complex

Nicolas Queyriaux,\* Jorge J. Cabrera-Trujillo, Nina Durvin, Laure Vendier, Karinne Miquieu\* and Antoine Simonneau\*

