

# Chemical Science

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## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 16(3) 983–1470 (2025)



**Cover**  
See Guozhong Xu, Xiuze Hei, Jing Li *et al.*, pp. 1106–1114. Image reproduced by permission of Xiuze Hei from *Chem. Sci.*, 2025, 16, 1106.



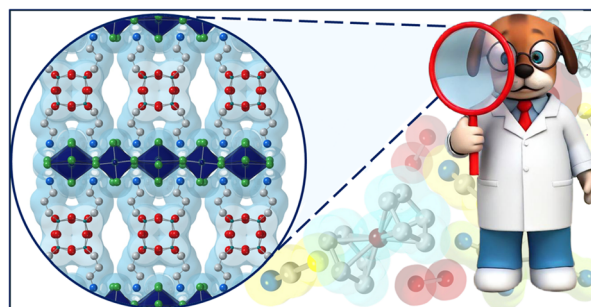
**Inside cover**  
See Himanshu Mishra *et al.*, pp. 1115–1125. Image reproduced by permission of KAUST from *Chem. Sci.*, 2025, 16, 1115.

## COMMENTARY

999

### A focus on microporous perovskites: new tricks for an old dog

Miriam Segundo-Osorio, A. Paulina Gómora-Figueroa and Diego Solís-Ibarra\*

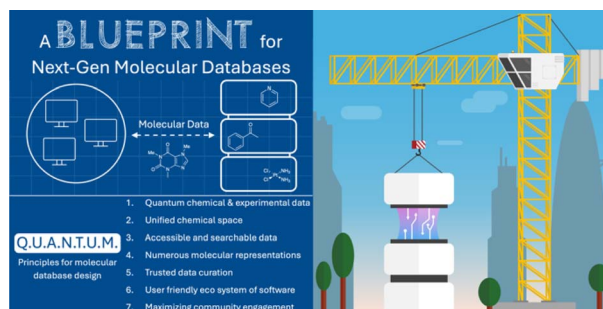


## PERSPECTIVES

1002

### Beyond chemical structures: lessons and guiding principles for the next generation of molecular databases

Timo Sommer, Cian Clarke and Max García-Melchor\*



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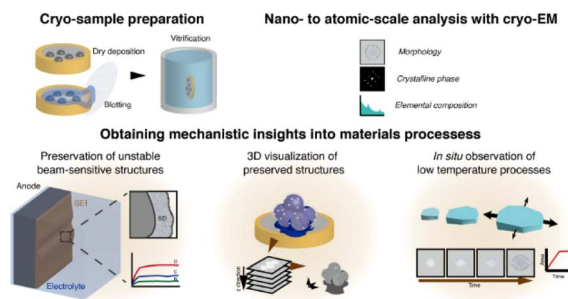
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## PERSPECTIVES

1017

## Unravelling complex mechanisms in materials processes with cryogenic electron microscopy

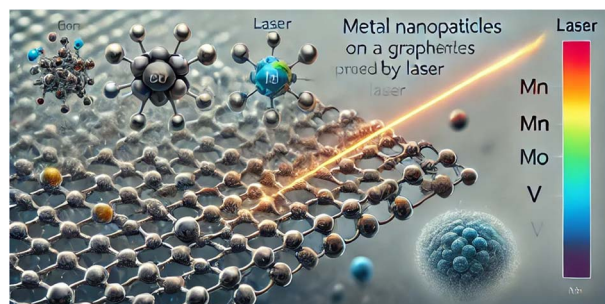
Minyoung Lee, Yongsoon Jeon, Sungin Kim, Ihnkyung Jung, Sungsu Kang, Seol-Ha Jeong\* and Jungwon Park\*



1036

## Unconventional aspects in metal-embedded laser-induced graphene

Arie Borenstein\* and Richard B. Kaner

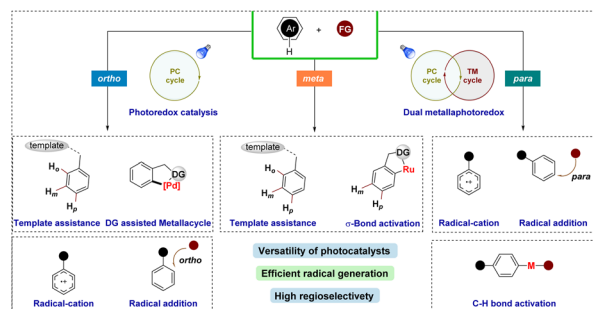


## REVIEWS

1041

## Photocatalytic regioselective C–H bond functionalizations in arenes

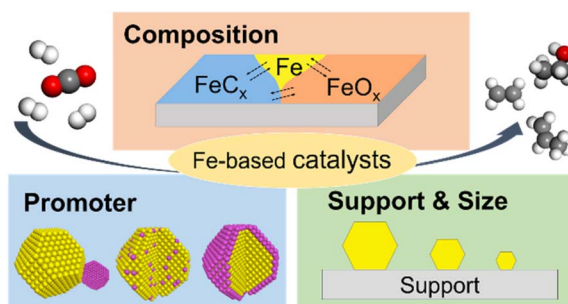
Jun Hu, Suman Pradhan, Satyadeep Waiba and Shoubhik Das\*



1071

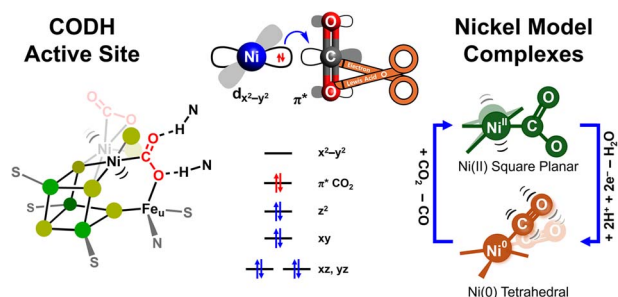
Structure–reactivity relationships in CO<sub>2</sub> hydrogenation to C<sub>2+</sub> chemicals on Fe-based catalysts

Jie Zhu, Shamil Shaikhutdinov\* and Beatriz Roldan Cuenya



## REVIEWS

1093

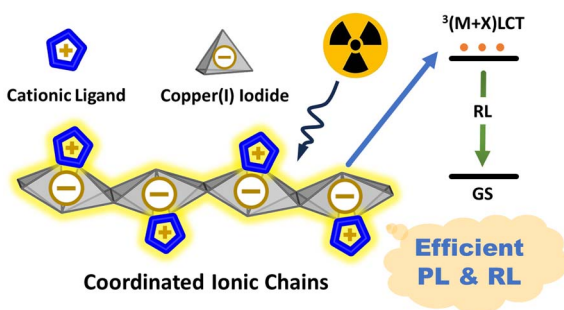


### Nickel model complexes to mimic carbon monoxide dehydrogenase reactions

Changho Yoo,\* Jonghoon Choi\* and Yunho Lee\*

## EDGE ARTICLES

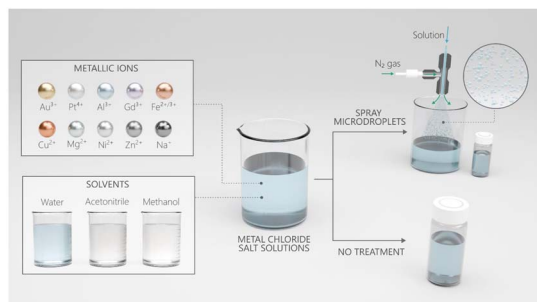
1106



### Strongly photoluminescent and radioluminescent copper(I) iodide hybrid materials made of coordinated ionic chains

Jingwen Chen, Kang Zhou, Jingbai Li, Guozhong Xu,\* Xiuze Hei\* and Jing Li\*

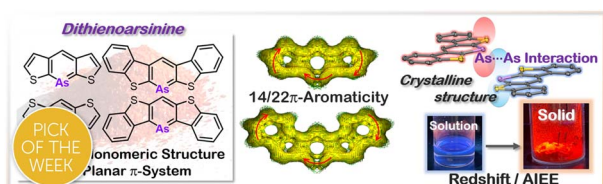
1115



### Why do some metal ions spontaneously form nanoparticles in water microdroplets? Disentangling the contributions of the air–water interface and bulk redox chemistry

Muzzamil Ahmad Eatoo, Nimer Wehbe, Najeh Kharbatia, Xianrong Guo and Himanshu Mishra\*

1126



### Dithienoarsinines: stable and planar $\pi$ -extended arsabenzenes

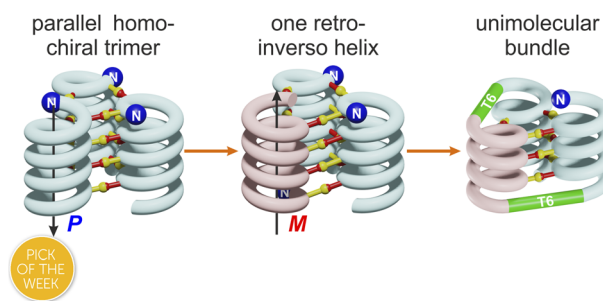
Akifumi Sumida, Akinori Saeki, Kyohei Matsuo, Kensuke Naka and Hiroaki Imoto\*



1136

**Design of an abiotic unimolecular three-helix bundle**

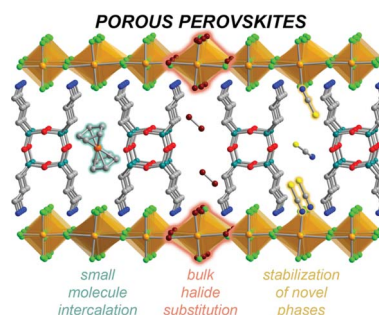
Shuhe Wang, Johannes Sigl, Lars Allmendinger, Victor Maurizot and Ivan Huc\*



1147

**Leveraging ordered voids in microporous perovskites for intercalation and post-synthetic modification**

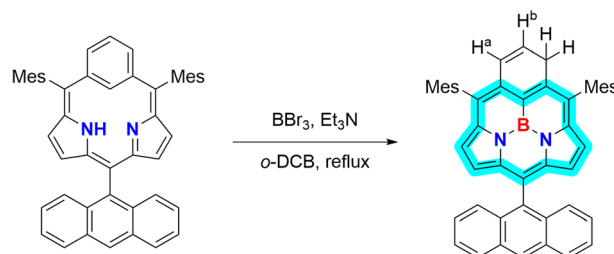
Connor W. Dalton, Paige M. Gannon, Werner Kaminsky and Douglas A. Reed\*



1155

**Sub-*m*-benzoporphyrin: a subcarbaporphyrinoid and its B<sup>III</sup> complex with an unprecedented planar tridentate 14π-aromatic network**

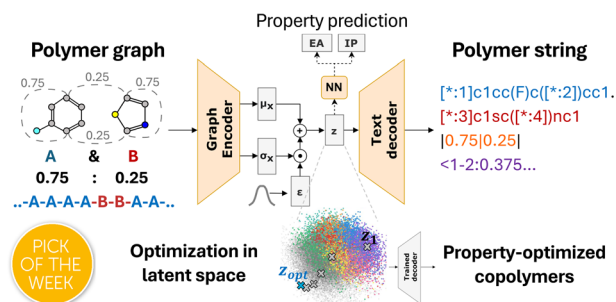
Le Liu, Shuangji Song, Jiyeon Lee, Yutao Rao, Ling Xu, Mingbo Zhou, Bangshao Yin, Juwon Oh, Jiwon Kim,\* Atsuhiko Osuka\* and Jianxin Song\*



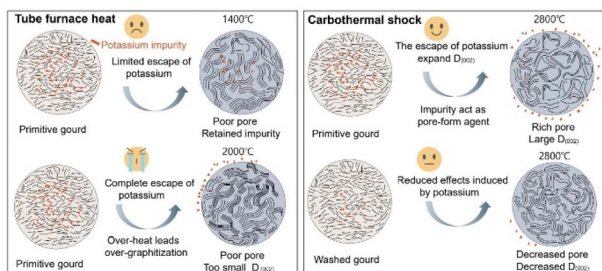
1161

**Inverse design of copolymers including stoichiometry and chain architecture**

Gabriel Vogel and Jana M. Weber\*



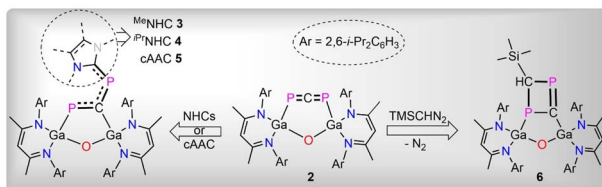
1179



## Potassium escaping balances the degree of graphitization and pore channel structure in hard carbon to boost plateau sodium storage capacity

Niubu LeGe, Ying-Hao Zhang, Wei-Hong Lai, Xiang-Xi He, Yun-Xiao Wang, Ling-fei Zhao, Min Liu,<sup>\*</sup> Xingqiao Wu<sup>\*</sup> and Shu-Lei Chou<sup>\*</sup>

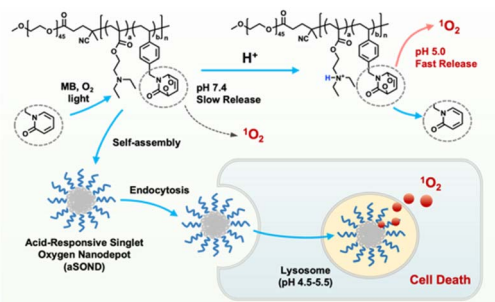
1189



## Synthesis and reactivity of a six-membered heterocyclic 1,3-diphosphaallene

Mahendra K. Sharma, Christoph Wölper, Hannah Siera, Gebhard Haberhauer and Stephan Schulz<sup>\*</sup>

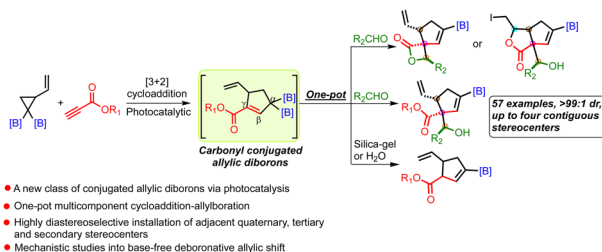
1197



## Acid-responsive singlet oxygen nanodepots

Zengwei Ran, Maolin Wang, Zhu Yuan, Yan Zhang,<sup>\*</sup> Guhuan Liu<sup>\*</sup> and Ronghua Yang<sup>\*</sup>

1205



## Strain-release enables access to carbonyl conjugated allylic diborons and alkenyl boronates having multiple contiguous stereocenters in a one-pot process

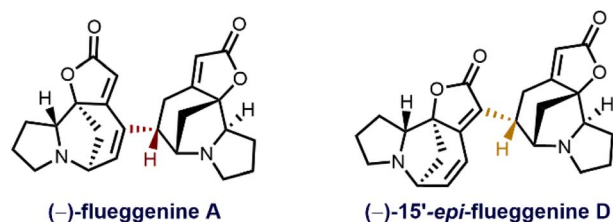
Het Vyas, Ashvin J. Gangani, Aiswarya Mini, Melissa Pathil, Austin Ruth and Abhishek Sharma<sup>\*</sup>



1216

**Total synthesis of (–)-flueggeine A and (–)-15'-epi-flueggeine D**

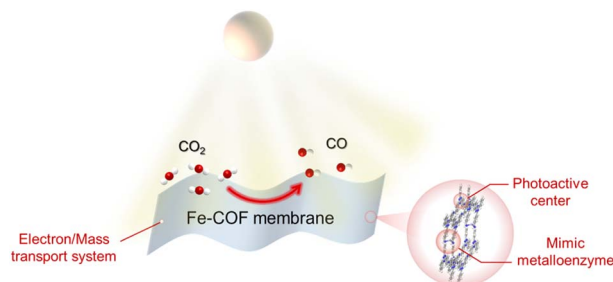
Seung Mo Seo, Dongwook Kim, Taewan Kim and Sunkyu Han\*



1222

**Mimic metalloenzymes with atomically dispersed Fe sites in covalent organic framework membranes for enhanced CO<sub>2</sub> photoreduction**

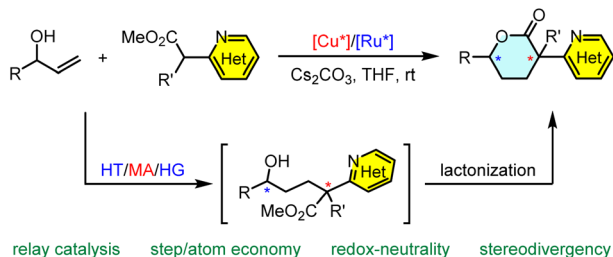
Shuaiqi Gao, Xiao Zhao, Qian Zhang, Linlin Guo, Zhiyong Li, Huiyong Wang,\* Suojiang Zhang and Jianji Wang\*



1233

**Stereodivergent assembly of  $\delta$ -valerolactones with an azaarene-containing quaternary stereocenter enabled by Cu/Ru relay catalysis**

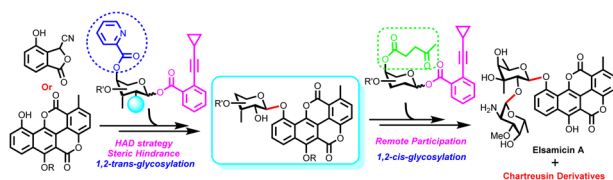
Kui Tian, Zhuan Jin, Xin-Lian Liu, Ling He, Hong-Fu Liu, Pin-Ke Yu, Xin Chang, Xiu-Qin Dong\* and Chun-Jiang Wang\*



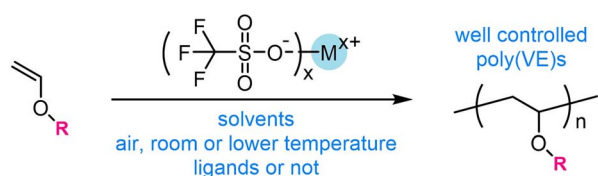
1241

**Collective total synthesis of chartreusin derivatives and bioactivity investigations**

Hong-Zhou Yi, Shu-Min Liang, Jing-Jing Li,\* Hui Liu, Jin-Xi Liao,\* De-Yong Liu, Qing-Ju Zhang, Ming-Zhong Cai\* and Jian-Song Sun\*



1250

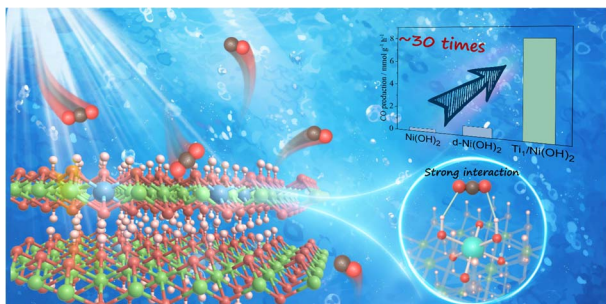


- ✓ Industrially available feedstocks
- ✓ High-molecular-weight poly(vinyl ether)s
- ✓ Tolerance to air and moisture
- ✓ Crystalline polymers with high tacticity

### Cationic polymerization of vinyl ethers using trifluoromethyl sulfonate/solvent/ligand to access well-controlled poly(vinyl ether)s

Liangyu Chen, Zhihao Wang, En Fang, Zhiqiang Fan and Shaofei Song\*

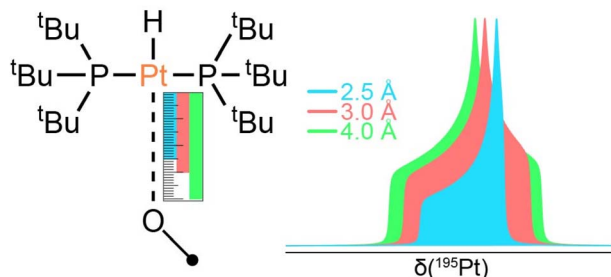
1265



### Electronic regulation of single-atomic Ti sites on metal hydroxide for boosting photocatalytic CO<sub>2</sub> reduction

Ning-Yu Huang, Bai Li, Duojie Wu, Di Chen, Yu-Tao Zheng, Bing Shao, Wenjuan Wang, Meng Gu, Lei Li\* and Qiang Xu\*

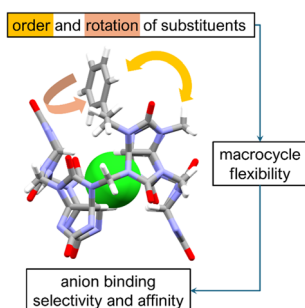
1271



### Structural characterization of surface immobilized platinum hydrides by sensitivity-enhanced <sup>195</sup>Pt solid state NMR spectroscopy and DFT calculations

Benjamin A. Atterberry, Erik J. Wimmer, Sina Klostermann, Wolfgang Frey, Johannes Kästner, Deven P. Estes\* and Aaron J. Rossini\*

1288



### Reversing selectivity of bambusuril macrocycles toward inorganic anions by installing spacious substituents on their portals

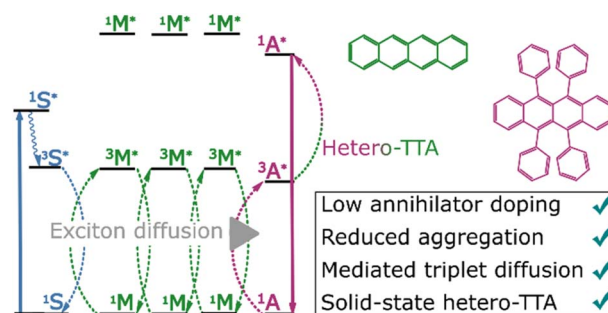
Carola Rando, Surbhi Grewal, Jan Sokolov, Petr Kulhánek\* and Vladimír Šindelář\*



1293

### Separating triplet exciton diffusion from triplet–triplet annihilation by the introduction of a mediator

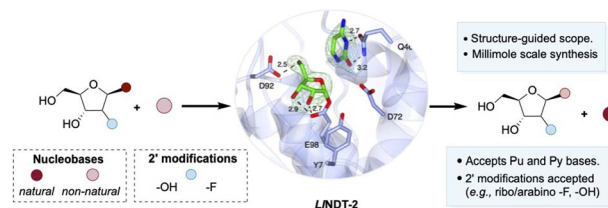
Andrew J. Carrod, Anton M. Berghuis, Vishnu Nair Gopalakrishnan, Andrew Monkman, Andrew Danos and Karl Börjesson\*



1302

### Biocatalytic synthesis of ribonucleoside analogues using nucleoside transglycosylase-2

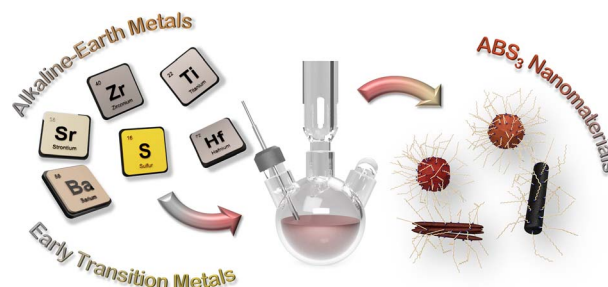
Admir Salihovic, Alex Ascham, Petja S. Rosenqvist, Andrea Taladriz-Sender, Paul A. Hoskisson, David R. W. Hodgson, Gideon Grogan\* and Glenn A. Burley\*



1308

### A reliable, colloidal synthesis method of the orthorhombic chalcogenide perovskite, BaZrS<sub>3</sub>, and related ABS<sub>3</sub> nanomaterials (A = Sr, Ba; B = Ti, Zr, Hf): a step forward for earth-abundant, functional materials

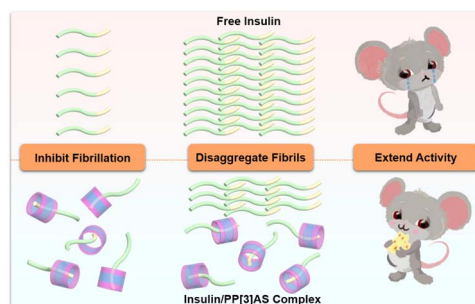
Daniel C. Hayes, Shubhanshu Agarwal, Kiruba Catherine Vincent, Izoduwa M. Aimiuwu, Apurva A. Pradhan, Madeleine C. Uible, Suzanne C. Bart and Rakesh Agrawal\*



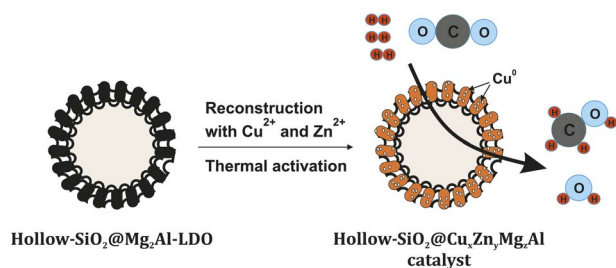
1321

### Efficient encapsulation of insulin by a giant macrocycle as a powerful approach to the inhibition of its fibrillation

Ruotong Wang, Zihan Fang, Shenghui Li, Ziliang Zhang, Ming Dong, Junyi Chen,\* Qingbin Meng\* and Chunju Li\*



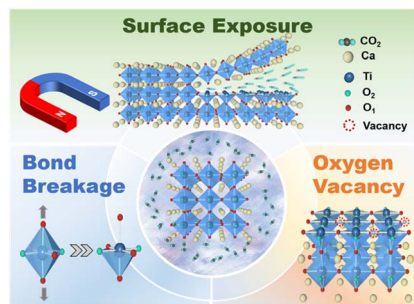
1327



### Hollow-SiO<sub>2</sub>@Cu<sub>x</sub>Zn<sub>y</sub>Mg<sub>z</sub>Al-LDHs as catalyst precursors for CO<sub>2</sub> hydrogenation to methanol

Tomasz Kondratowicz, Marta Gajewska, Jiangtong Li, Molly Meng-Jung Li, Zoë R. Turner, Chunping Chen\* and Dermot O'Hare\*

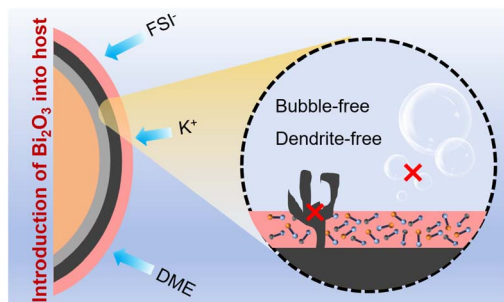
1336



### CO<sub>2</sub>-broken Ti–O bonds in the TiO<sub>6</sub> octahedron of CaTiO<sub>3</sub> for greatly enhanced room-temperature ferromagnetism

Yuqi Ouyang, Bo Gao, Yaozheng Tang, Lianyu Li and Qun Xu\*

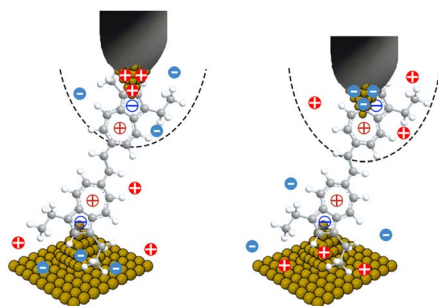
1344



### A bismuth oxide-modified copper host achieving bubble-free and stable potassium metal batteries

Guokai Shi, Junpeng Xie, Zhibin Li, Peng Sun, Ying Yin, Likun Pan, Kwun Nam Hui, Wenjie Mai and Jinliang Li\*

1353



### Switchable modes of azulene-based single molecule–electrode coupling controlled by interfacial charge distribution

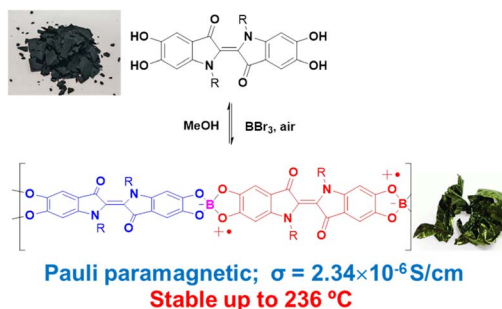
Chengyang Zhang, Yaqi Kong, Junjun Xiang, Sikang Chen, Alexei. A. Kornyshev, Jens Ulstrup, Xike Gao,\* Guangping Zhang,\* Yueqi Li\* and Jinghong Li\*



1364

### A recyclable dynamic semiconducting polymer consisting of Pauli-paramagnetic diradicaloids promoted and stabilized by catechol–boron coordination

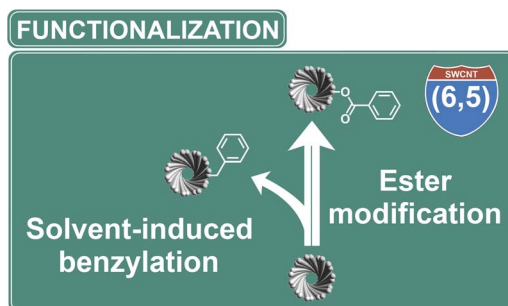
Youbing Mu,\* Chenxi Xiong, Minghui Cui, Mingxu Sun, Xinyu Chen, Biao Xiao, Hongqian Sang, Zhenxing Wang, Hangxu Liu, Zhenggang Lan, You Song\* and Xiaobo Wan\*



1374

### Unraveling aryl peroxide chemistry to enrich optical properties of single-walled carbon nanotubes

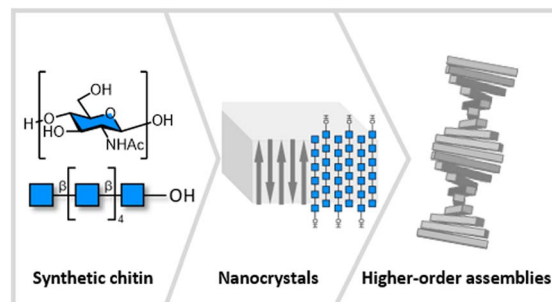
Patrycja Taborowska, Andrzej Dzieńia\* and Dawid Janas\*



1390

### Synthetic chitin oligosaccharide nanocrystals and their higher-order assemblies

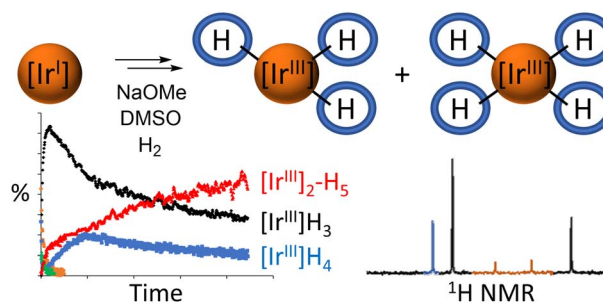
Surusch Djalali, Yun Jing, Yu Ogawa\* and Martina Delbianco\*



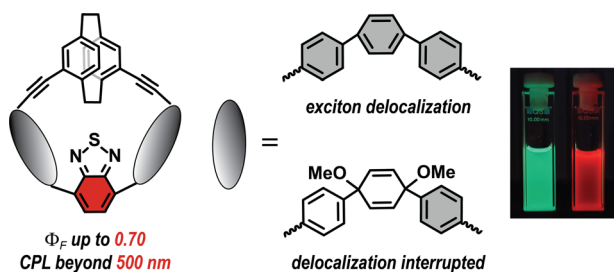
1396

### Iridium trihydride and tetrahydride complexes and their role in catalytic polarisation transfer from parahydrogen to pyruvate

Ben. J. Tickner and Simon B. Duckett\*



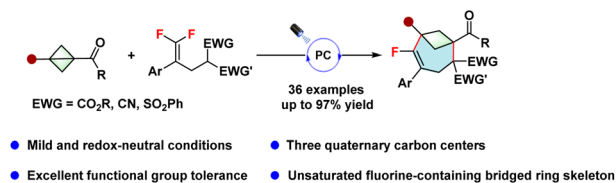
1405



### Role of exciton delocalization in chiroptical properties of benzothiadiazole carbon nano hoops

Kovida Kovida, Juraj Malinčík, Carlos M. Cruz, Araceli G. Campaña and Tomáš Šolomek\*

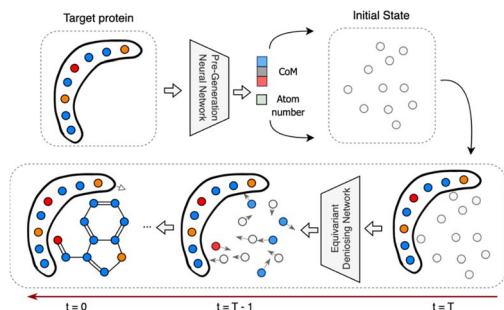
1411



### Synthesis of fluorine-containing bicyclo[4.1.1]octenes via photocatalyzed defluorinative (4 + 3) annulation of bicyclo[1.1.0]butanes with gem-difluoroalkenes

Kuan Zhang, Zhengyang Gao, Yan Xia, Pengfei Li, Pin Gao, Xin-Hua Duan and Li-Na Guo\*

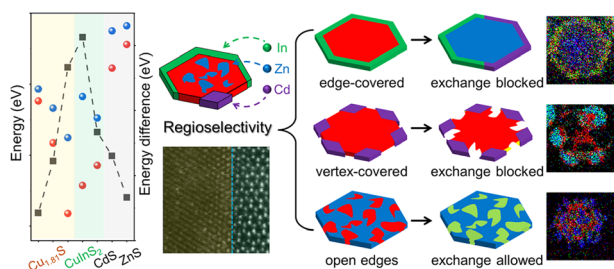
1417



### DiffBP: generative diffusion of 3D molecules for target protein binding

Haitao Lin, Yufei Huang, Odin Zhang, Siqi Ma, Meng Liu, Xuanjing Li, Lirong Wu, Jishui Wang, Tingjun Hou\* and Stan Z. Li\*

1432



### Determinants of regioreselectivity of heterostructures in cation exchange reactions

Xuelian Qu, Huisheng Zhang, Tianyi Gao, Fei Zhang, Ying Zhang, Ding-Jiang Xue and Yang Liu\*

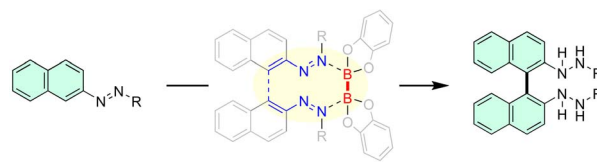


## EDGE ARTICLES

1441

**Reductive coupling of azonaphthalenes for the synthesis of BINAMs via a diboron-enabled [5,5]-sigmatropic rearrangement**

Liang-Wen Qi, Emmanuella Bema Twumasi, Xiao-Wei Li, Rui Li and Yixin Lu\*

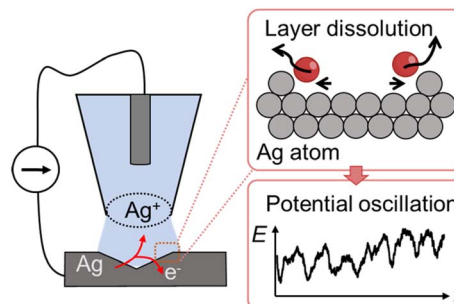


- ◆ Transition metal & oxidant free
- ◆ New mechanism
- ◆ Chem- & regioselectivities
- ◆ Mild reaction conditions
- ◆ No chromatography
- ◆ Scalability, >10 g

1447

**Kinetics and dynamics of atomic-layer dissolution on low-defect Ag**

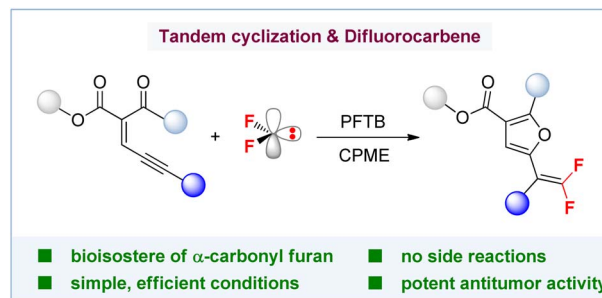
Yufei Wang, Roberto Garcia-Carrillo and Hang Ren\*



1455

**General access to furan-substituted *gem*-difluoroalkenes enabled by PFTB-promoted cross-coupling of ene-yne-ketones and difluorocarbene**

Na Li, Chenghui Li, Qianying Zhou, Xin Zhang, Zhouming Deng, Zhong-Xing Jiang and Zhigang Yang\*



- bioisostere of  $\alpha$ -carbonyl furan
- no side reactions
- simple, efficient conditions
- potent antitumor activity

## CORRECTIONS

1465

**Correction: Enhanced catalytic activity of solubilised species obtained by counter-cation exchange of K  $\{Co^{II}_{1.5}[Fe^{II}(CN)_6]\}$  for water oxidation**

Yusuke Seki, Takashi Nakazono, Hiroyasu Tabe and Yusuke Yamada\*



## CORRECTIONS

1467

**Correction: FragGen: towards 3D geometry reliable fragment-based molecular generation**

Odin Zhang, Yufei Huang, Shicheng Chen, Mengyao Yu, Xujun Zhang, Haitao Lin, Yundian Zeng, Mingyang Wang, Zhenxing Wu, Huifeng Zhao, Zaixi Zhang, Chenqing Hua, Yu Kang, Sunliang Cui,\* Peichen Pan,\* Chang-Yu Hsieh\* and Tingjun Hou\*

