

# Chemical Science

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## IN THIS ISSUE

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



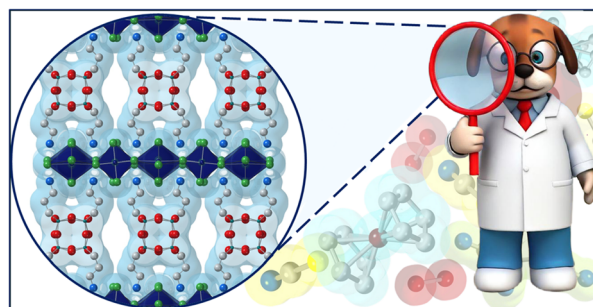
**Inside cover**  
See Himanshu Mishra *et al.*, pp. 1115–1125. Image reproduced by permission of KAUST from *Chem. Sci.*, 2025, 16, 1115.

## COMMENTARY

999

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

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

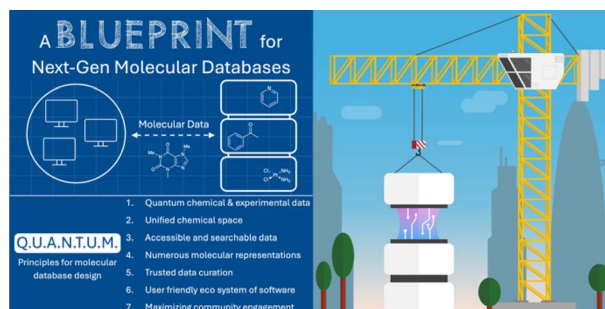


## PERSPECTIVES

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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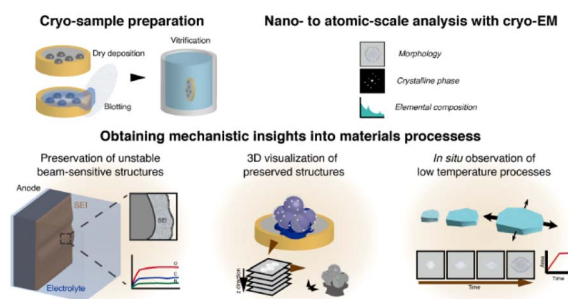
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## PERSPECTIVES

1017

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

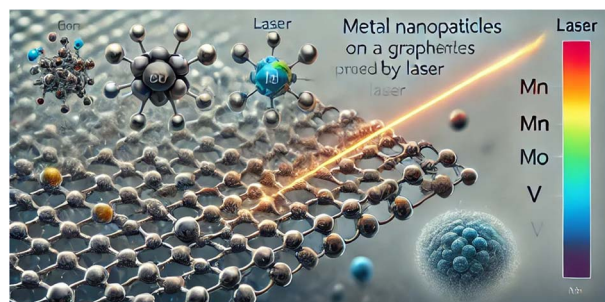
Minyoung Lee, Yongsoon Jeon, Sungjin Kim, Ihnkyung Jung, Sungsu Kang, Seol-Ha Jeong\* and Jungwon Park\*



1036

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

Arie Borenstein\* and Richard B. Kaner

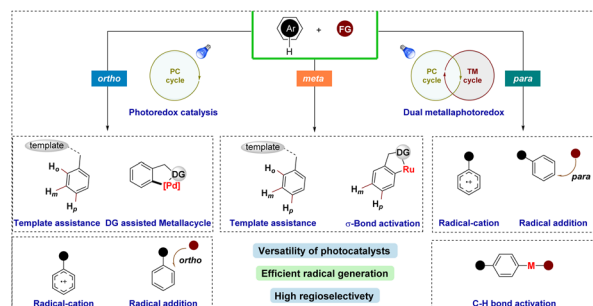


## REVIEWS

1041

## Photocatalytic regioselective C–H bond functionalizations in arenes

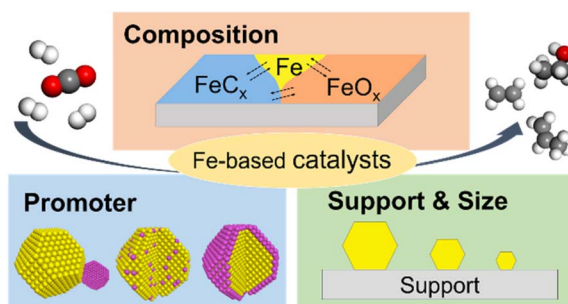
Jun Hu, Suman Pradhan, Satyadeep Waiba and Shoubhik Das\*



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

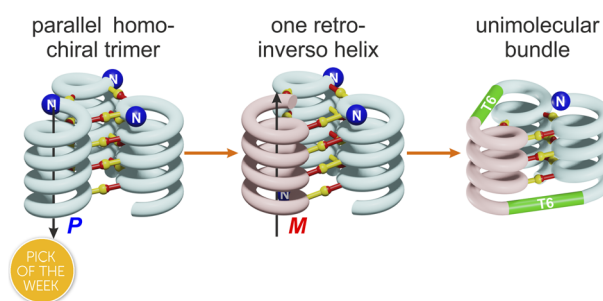




1136

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

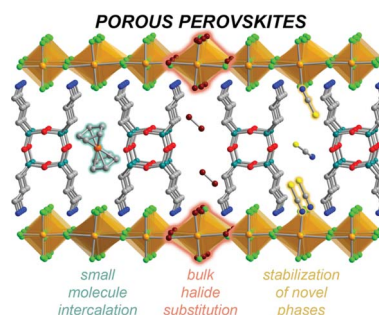
Shuhe Wang, Johannes Sigl, Lars Allmendinger, Victor Maurizot and Ivan Huc\*



1147

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

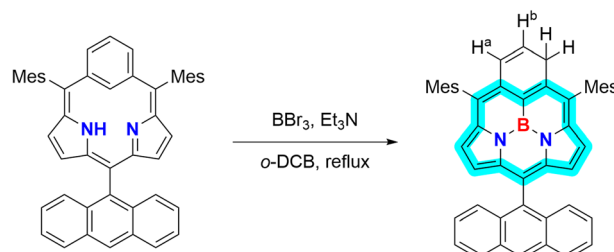
Connor W. Dalton, Paige M. Gannon, Werner Kaminsky and Douglas A. Reed\*



1155

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

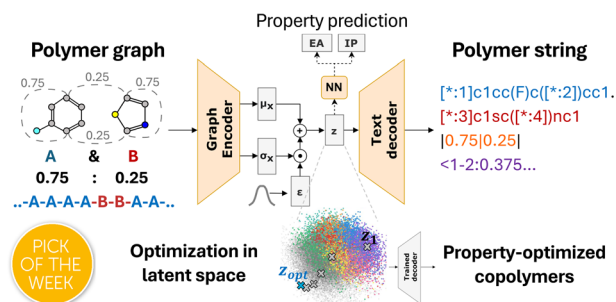
Le Liu, Shuangji Song, Jiyeon Lee, Yutao Rao, Ling Xu, Mingbo Zhou, Bangshao Yin, Juwon Oh, Jiwon Kim,\* Atsuhiko Osuka\* and Jianxin Song\*



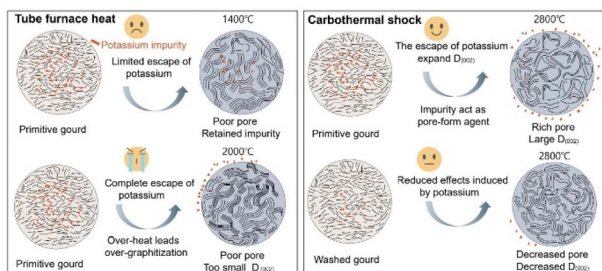
1161

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

Gabriel Vogel and Jana M. Weber\*



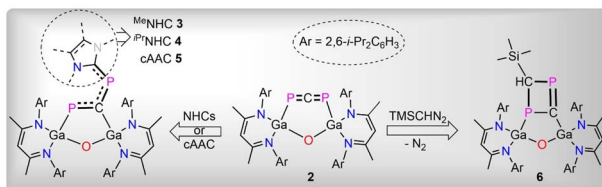
1179



## 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>

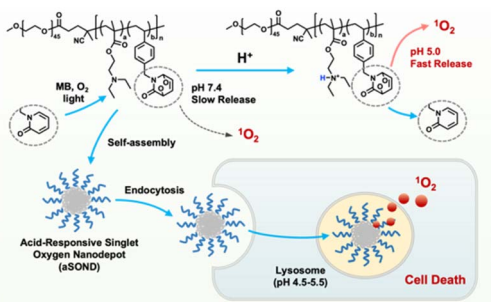
1189



## 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>

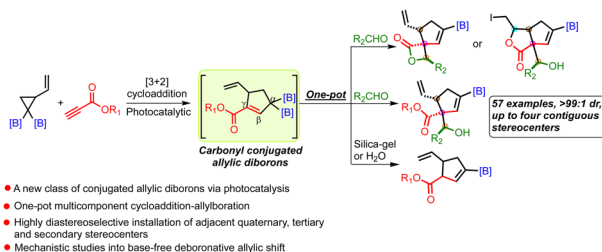
1197



## 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



- A new class of conjugated allylic diborons via photocatalysis
- One-pot multicomponent cycloaddition-allylboration
- Highly diastereoselective installation of adjacent quaternary, tertiary and secondary stereocenters
- Mechanistic studies into base-free deboronative allylic shift

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

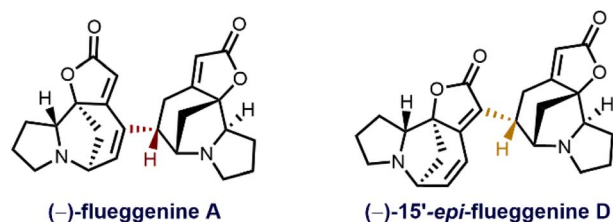
Het Vyas, Ashvin J. Gangani, Aiswarya Mini, Melissa Pathil, Austin Ruth and Abhishek Sharma<sup>\*</sup>



1216

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

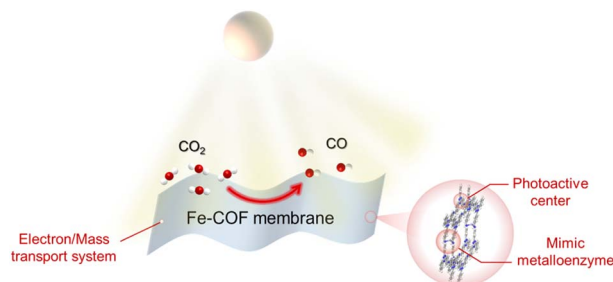
Seung Mo Seo, Dongwook Kim, Taewan Kim and Sunkyu Han\*



1222

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

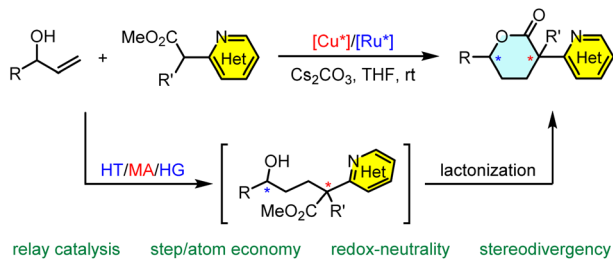
Shuaiqi Gao, Xiao Zhao, Qian Zhang, Linlin Guo, Zhiyong Li, Huiyong Wang,\* Suojiang Zhang and Jianji Wang\*



1233

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

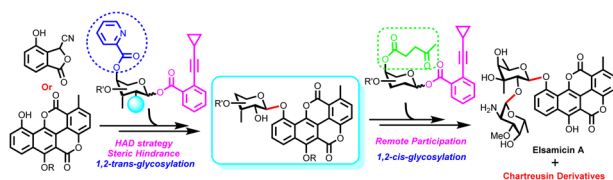
Kui Tian, Zhuan Jin, Xin-Lian Liu, Ling He, Hong-Fu Liu, Pin-Ke Yu, Xin Chang, Xiu-Qin Dong\* and Chun-Jiang Wang\*



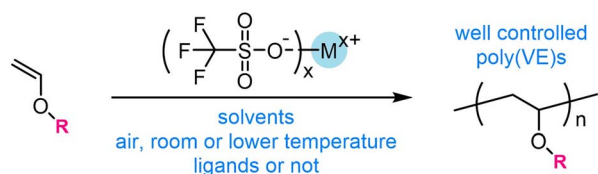
1241

**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

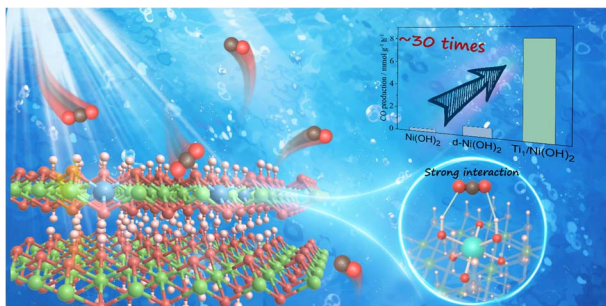


- ✓ Industrially available feedstocks
- ✓ High-molecular-weight poly(vinyl ether)s
- ✓ Tolerance to air and moisture
- ✓ Crystalline polymers with high tacticity

### 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\*

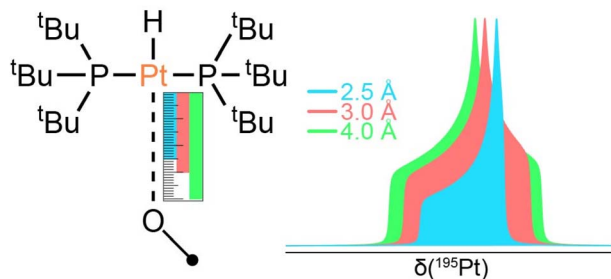
1265



### 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\*

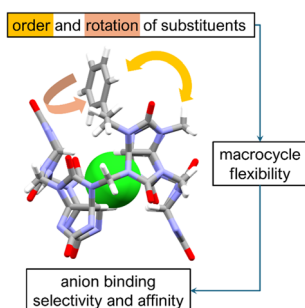
1271



### 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

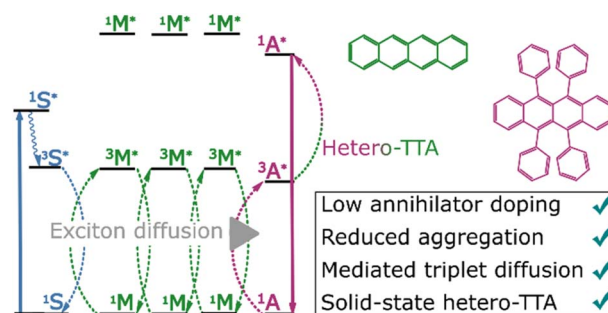
Carola Rando, Surbhi Grewal, Jan Sokolov, Petr Kulhánek\* and Vladimír Šindelář\*



1293

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

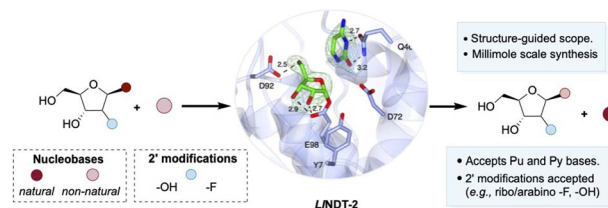
Andrew J. Carrod, Anton M. Berghuis, Vishnu Nair Gopalakrishnan, Andrew Monkman, Andrew Danos and Karl Börjesson\*



1302

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

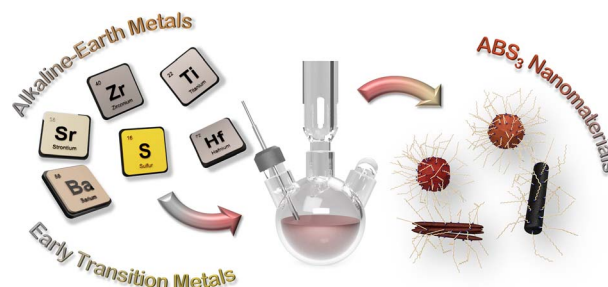
Admir Salihovic, Alex Ascham, Petja S. Rosenqvist, Andrea Taladriz-Sender, Paul A. Hoskisson, David R. W. Hodgson, Gideon Grogan\* and Glenn A. Burley\*



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

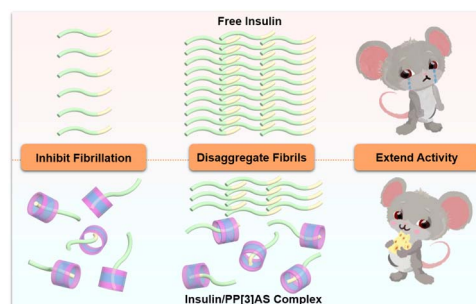
Daniel C. Hayes, Shubhanshu Agarwal, Kiruba Catherine Vincent, Izoduwa M. Aimiuwu, Apurva A. Pradhan, Madeleine C. Uible, Suzanne C. Bart and Rakesh Agrawal\*



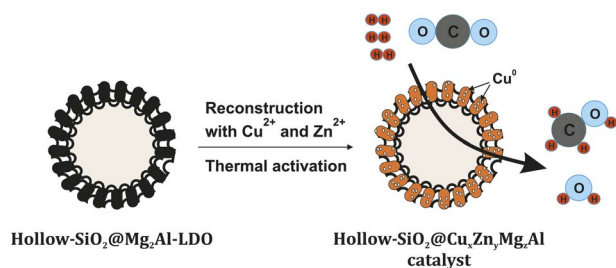
1321

### 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\*



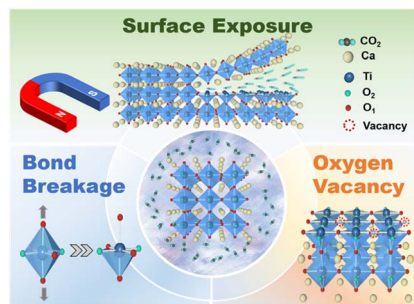
1327



### 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\*

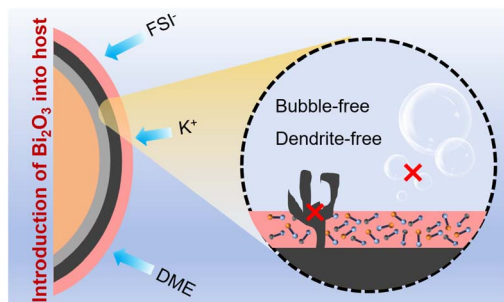
1336



### 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\*

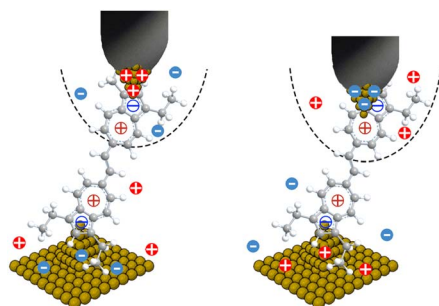
1344



### 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

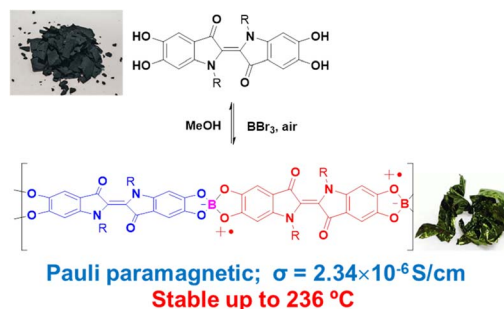
Chengyang Zhang, Yaqi Kong, Junjun Xiang, Sikang Chen, Alexei. A. Kornyshev, Jens Ulstrup, Xike Gao,\* Guangping Zhang,\* Yueqi Li\* and Jinghong Li\*



1364

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

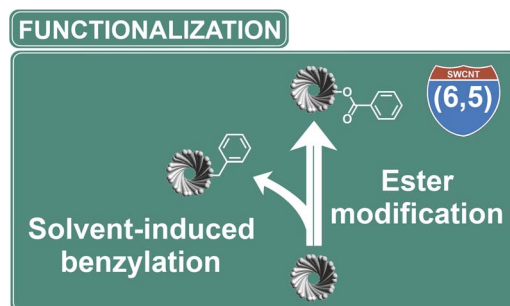
Youbing Mu,\* Chenxi Xiong, Minghui Cui, Mingxu Sun, Xinyu Chen, Biao Xiao, Hongqian Sang, Zhenxing Wang, Hangxu Liu, Zhenggang Lan, You Song\* and Xiaobo Wan\*



1374

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

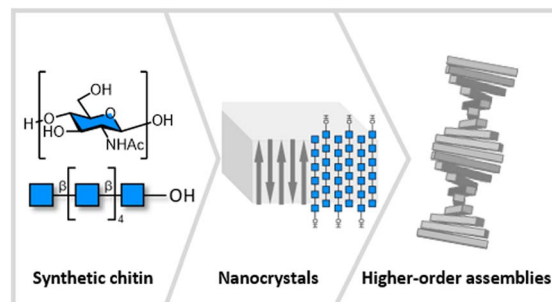
Patrycja Taborowska, Andrzej Dzieńia\* and Dawid Janas\*



1390

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

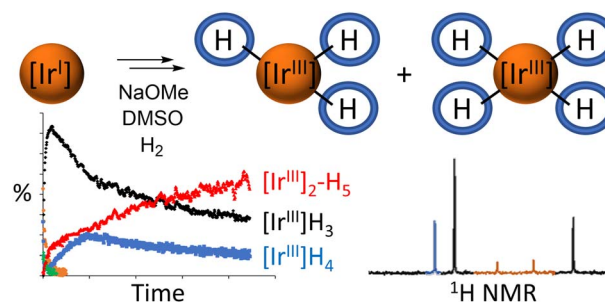
Surusch Djalali, Yun Jing, Yu Ogawa\* and Martina Delbianco\*



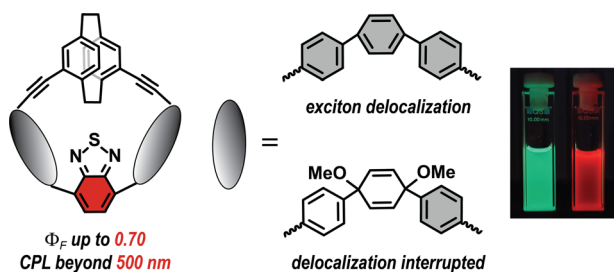
1396

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

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



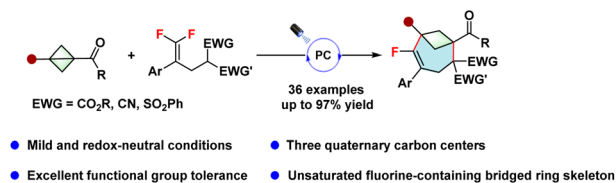
1405



### 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\*

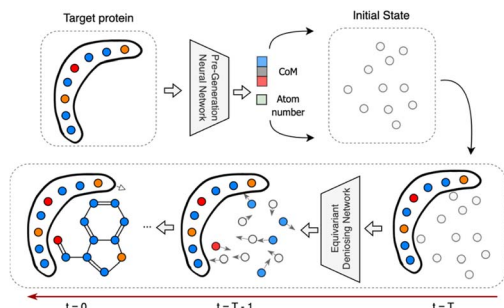
1411



### 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\*

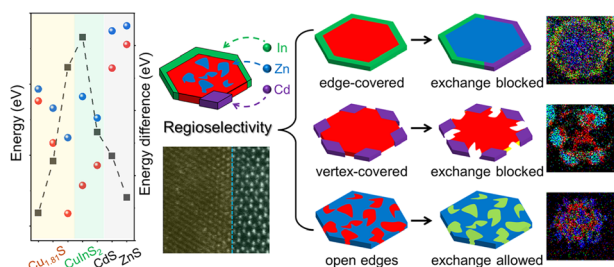
1417



### 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 regioselectivity of heterostructures in cation exchange reactions

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

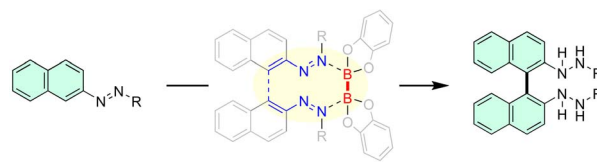


## EDGE ARTICLES

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\*

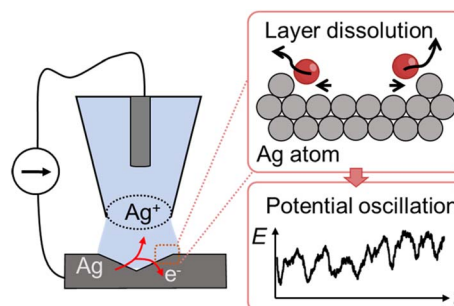


- ◆ Transition metal & oxidant free
- ◆ New mechanism
- ◆ Chem- & regioselectivities
- ◆ Mild reaction conditions
- ◆ No chromatography
- ◆ Scalability, >10 g

1447

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

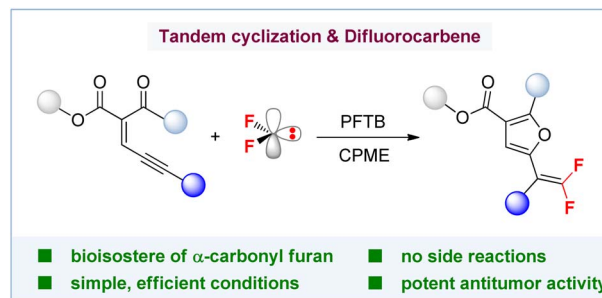
Yufei Wang, Roberto Garcia-Carrillo and Hang Ren\*



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\*



## 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\*

