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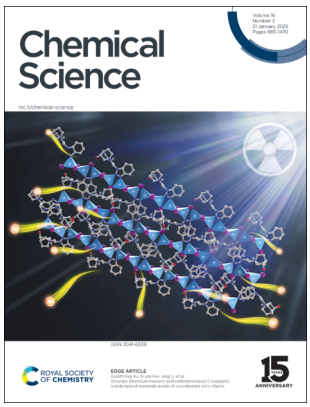
IN THIS ISSUE

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



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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.

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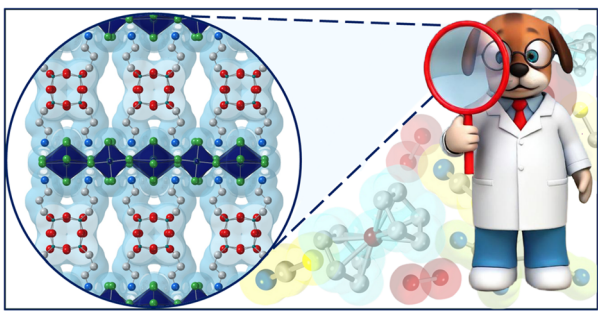
A focus on microporous perovskites: new tricks for an old dog

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



PERSPECTIVES

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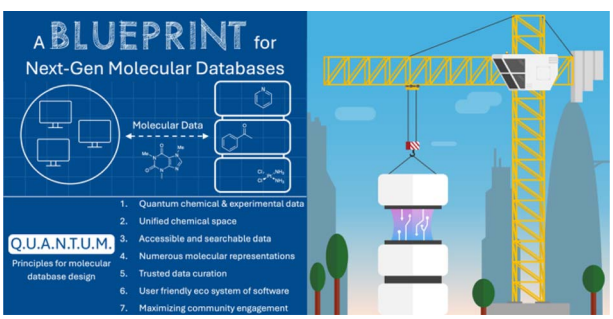
Beyond chemical structures: lessons and guiding principles for the next generation of molecular databases

Timo Sommer, Cian Clarke and Max García-Melchor*



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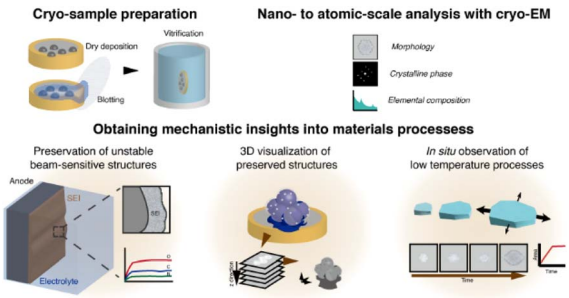
Unravelling complex mechanisms in materials processes with cryogenic electron microscopy

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



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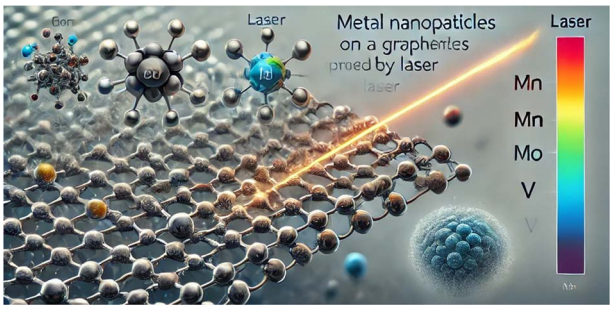
Unconventional aspects in metal-embedded laser-induced graphene

Arie Borenstein* and Richard B. Kaner



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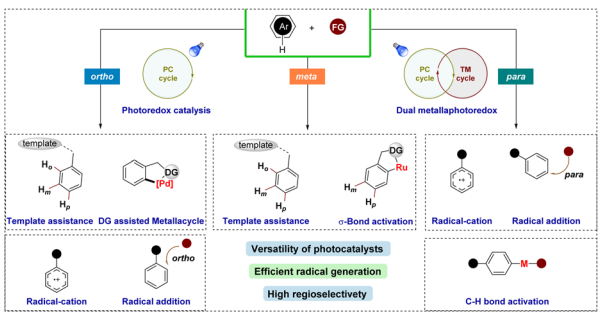
Photocatalytic regioselective C–H bond functionalizations in arenes

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



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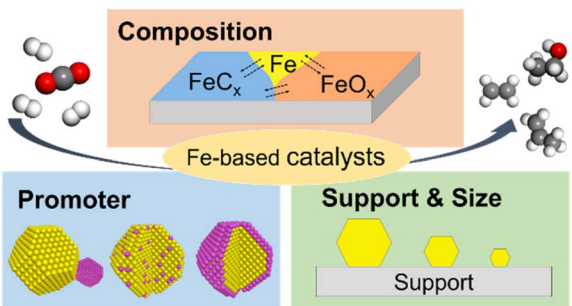
Structure–reactivity relationships in CO_2 hydrogenation to C_{2+} chemicals on Fe-based catalysts

Jie Zhu, Shamil Shaikhutdinov* and Beatriz Roldan Cuenya



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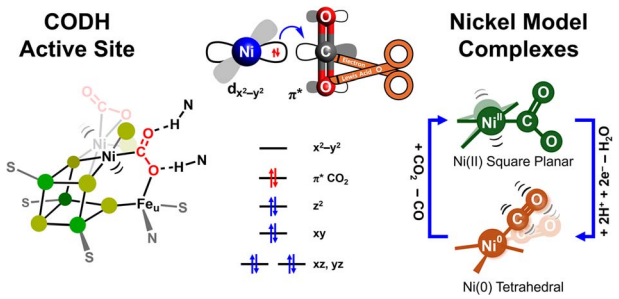

Nickel model complexes to mimic carbon monoxide dehydrogenase reactions

Changho Yoo,* Jonghoon Choi* and Yunho Lee*

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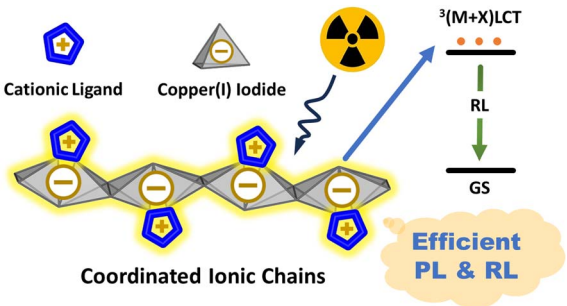

Strongly photoluminescent and radioluminescent copper(I) iodide hybrid materials made of coordinated ionic chains

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

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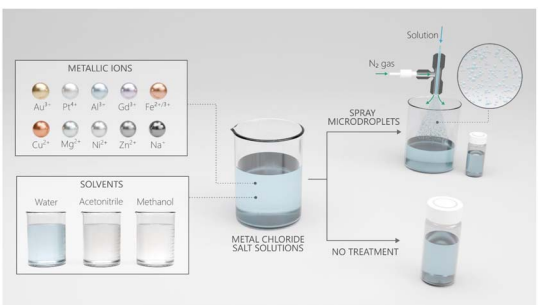

Why do some metal ions spontaneously form nanoparticles in water microdroplets? Disentangling the contributions of the air–water interface and bulk redox chemistry

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

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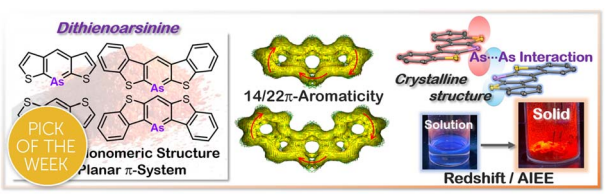

Dithienoarsinines: stable and planar π-extended arsabenzenes

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

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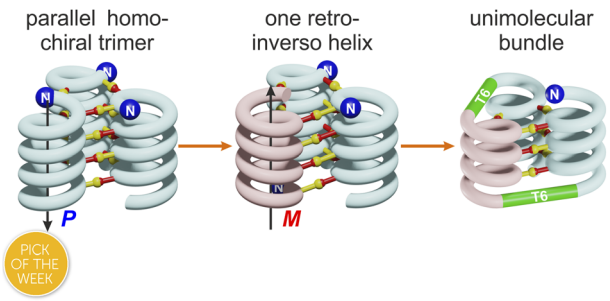
Design of an abiotic unimolecular three-helix bundle

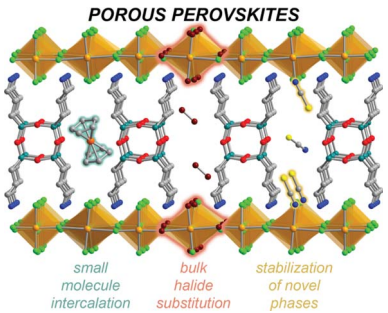
Shuhe Wang, Johannes Sigl, Lars Allmendinger, Victor Maurizot and Ivan Huc*



1147

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

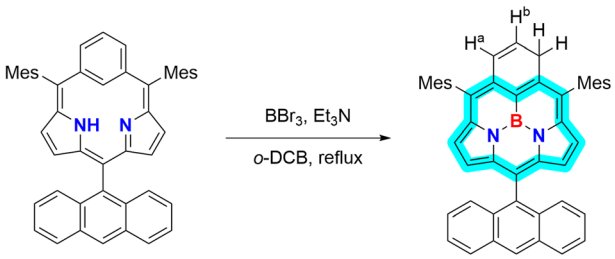
Connor W. Dalton, Paige M. Gannon, Werner Kaminsky and Douglas A. Reed*



1155

Sub-*m*-benziporphyrin: a subcarbaporphyrinoid and its B^{III} complex with an unprecedented planar tridentate 14π-aromatic network

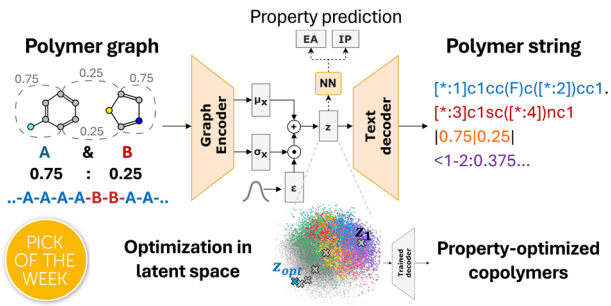
Le Liu, Shuangji Song, Jiyeon Lee, Yutao Rao, Ling Xu, Mingbo Zhou, Bangshao Yin, Juwon Oh, Jiwon Kim,* Atsuhiro Osuka* and Jianxin Song*



1161

Inverse design of copolymers including stoichiometry and chain architecture

Gabriel Vogel and Jana M. Weber*



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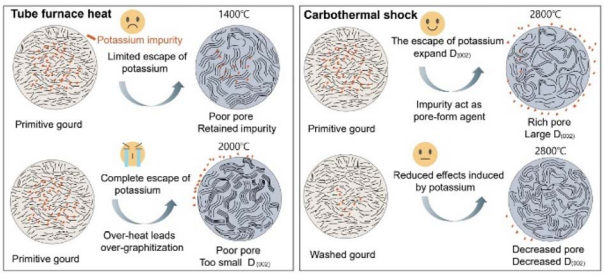

Potassium escaping balances the degree of graphitization and pore channel structure in hard carbon to boost plateau sodium storage capacity

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

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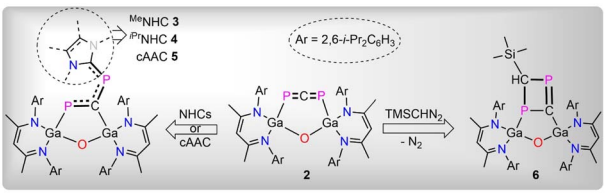

Synthesis and reactivity of a six-membered heterocyclic 1,3-diphosphaallene

Mahendra K. Sharma, Christoph Wölper, Hannah Siera, Gebhard Haberhauer and Stephan Schulz*

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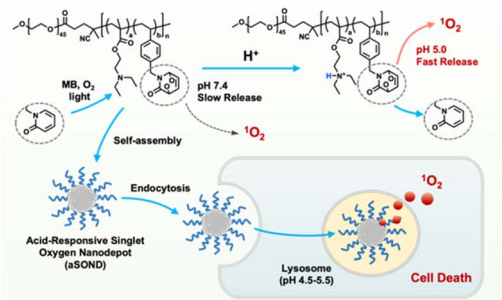

Acid-responsive singlet oxygen nanodepots

Zengwei Ran, Maolin Wang, Zhu Yuan, Yan Zhang,* Guhuan Liu* and Ronghua Yang*

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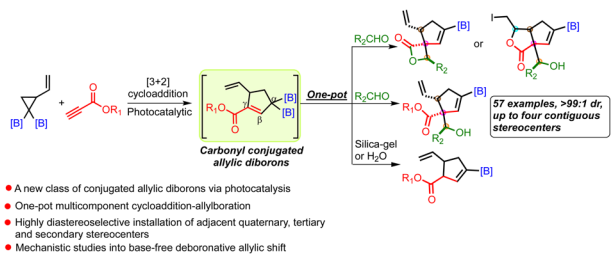

Strain-release enables access to carbonyl conjugated allylic diborons and alkenyl boronates having multiple contiguous stereocenters in a one-pot process

Het Vyas, Ashvin J. Gangani, Aiswarya Mini, Melissa Pathil, Austin Ruth and Abhishek Sharma*

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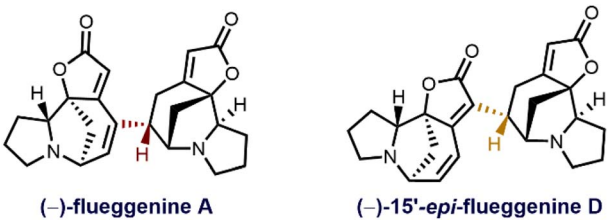
Total synthesis of (−)-flueggenine A and (−)-15′-*epi*-flueggenine D

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



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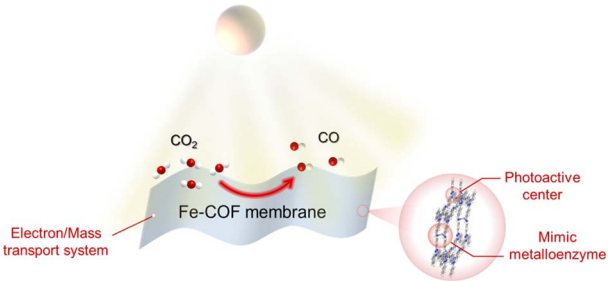
Mimic metalloenzymes with atomically dispersed Fe sites in covalent organic framework membranes for enhanced CO_2 photoreduction

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



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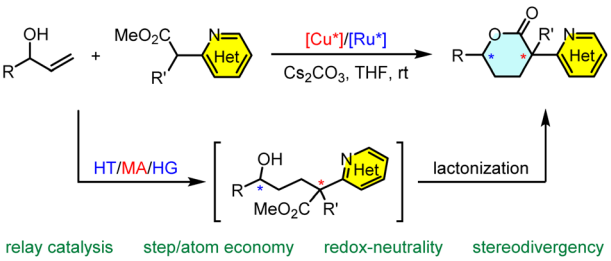
Stereodivergent assembly of δ-valerolactones with an azaarene-containing quaternary stereocenter enabled by Cu/Ru relay catalysis

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



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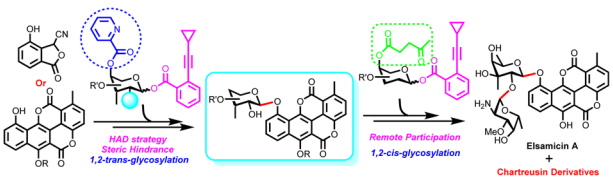
Collective total synthesis of chartreusin derivatives and bioactivity investigations

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*



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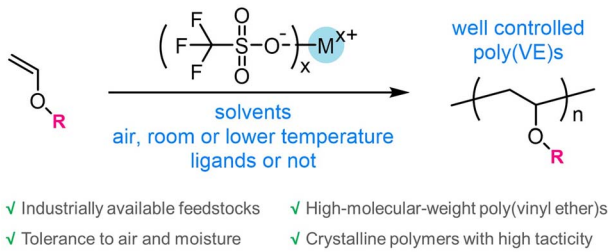

Cationic polymerization of vinyl ethers using trifluoromethyl sulfonate/solvent/ligand to access well-controlled poly(vinyl ether)s

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

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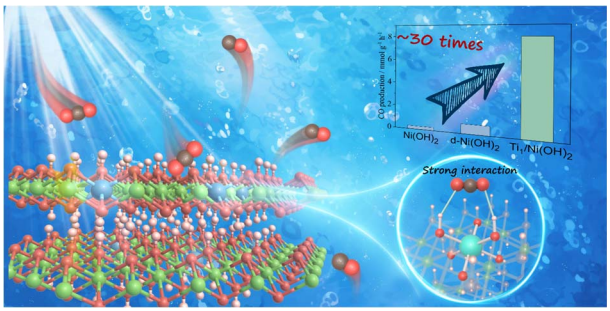

Electronic regulation of single-atomic Ti sites on metal hydroxide for boosting photocatalytic CO_2 reduction

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

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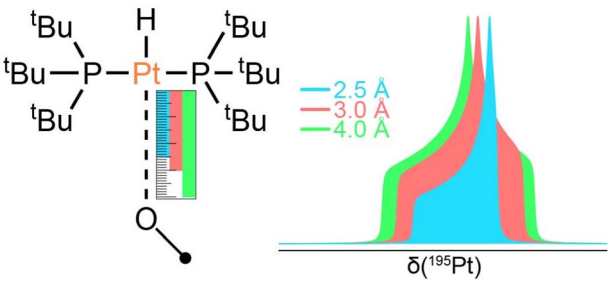

Structural characterization of surface immobilized platinum hydrides by sensitivity-enhanced ^{195}Pt solid state NMR spectroscopy and DFT calculations

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

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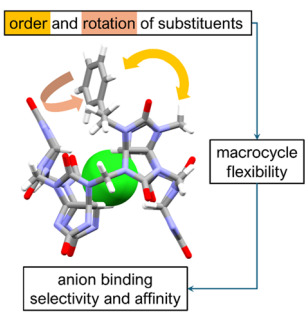

Reversing selectivity of bambusuril macrocycles toward inorganic anions by installing spacious substituents on their portals

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

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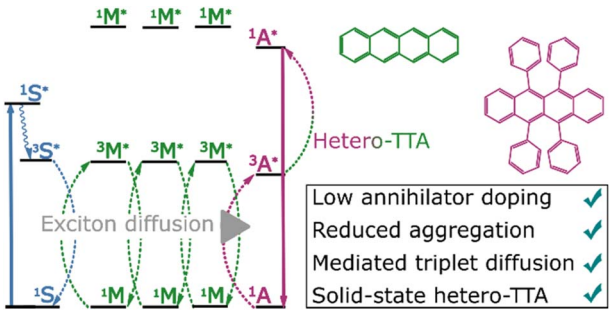
Separating triplet exciton diffusion from triplet–triplet annihilation by the introduction of a mediator

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



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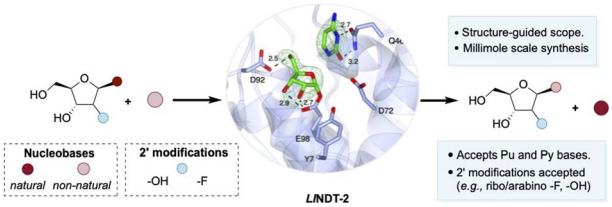
Biocatalytic synthesis of ribonucleoside analogues using nucleoside transglycosylase-2

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



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A reliable, colloidal synthesis method of the orthorhombic chalcogenide perovskite, $BaZrS_3$, and related ABS_3 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*

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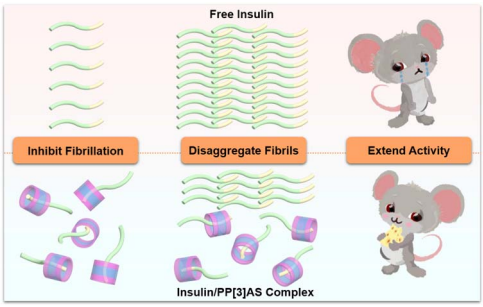
Efficient encapsulation of insulin by a giant macrocycle as a powerful approach to the inhibition of its fibrillation

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



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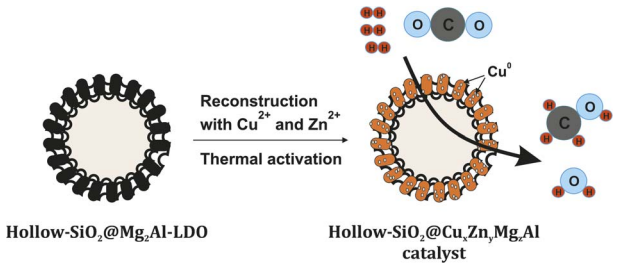

Hollow-SiO_2@$Cu_xZn_yMg_zAl$-LDHs as catalyst precursors for CO_2 hydrogenation to methanol

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

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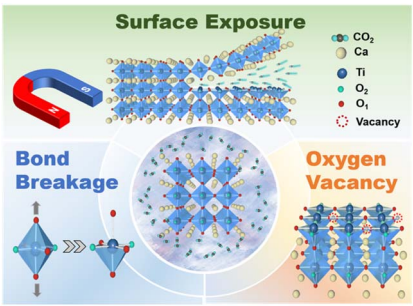

CO_2-broken Ti–O bonds in the TiO_6 octahedron of $CaTiO_3$ for greatly enhanced room-temperature ferromagnetism

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

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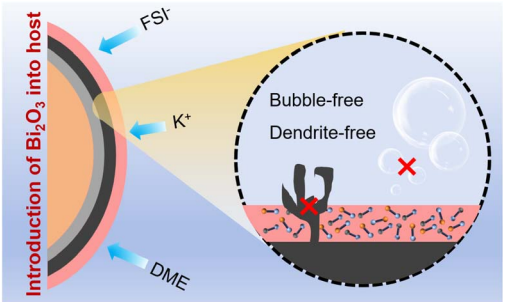

A bismuth oxide-modified copper host achieving bubble-free and stable potassium metal batteries

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

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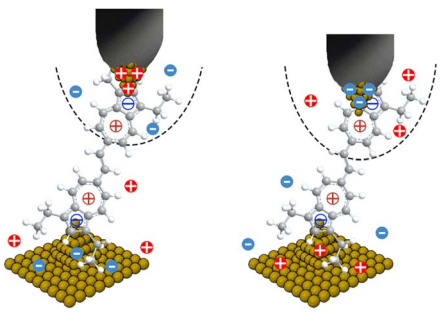

Switchable modes of azulene-based single molecule–electrode coupling controlled by interfacial charge distribution

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

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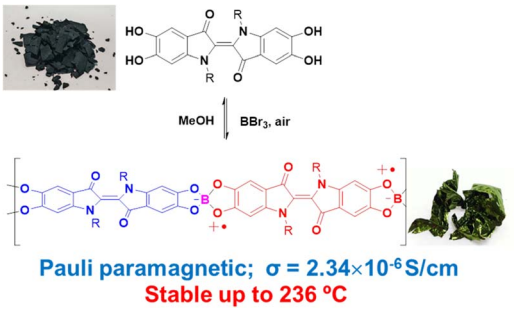
A recyclable dynamic semiconducting polymer consisting of Pauli-paramagnetic diradicaloids promoted and stabilized by catechol–boron coordination

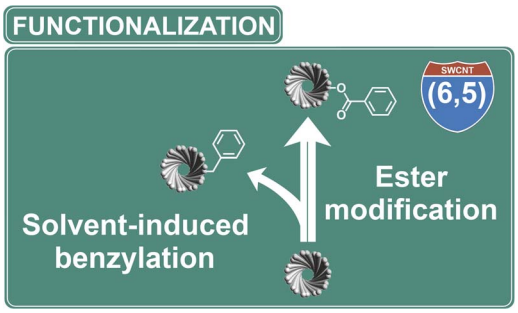
Youbing Mu,* Chenxi Xiong, Minghui Cui, Mingxu Sun, Xinyu Chen, Biao Xiao, Hongqian Sang, Zhenxing Wang, Hangxu Liu, Zhenggang Lan, You Song* and Xiaobo Wan*



1374

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

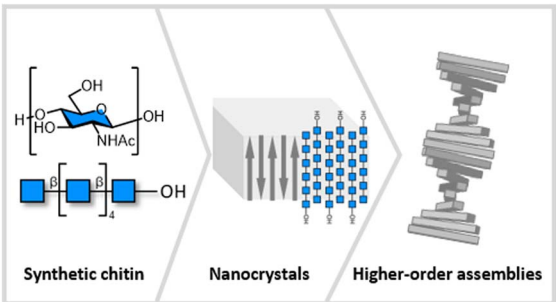
Patrycja Taborowska, Andrzej Dzienia* and Dawid Janas*



1390

Synthetic chitin oligosaccharide nanocrystals and their higher-order assemblies

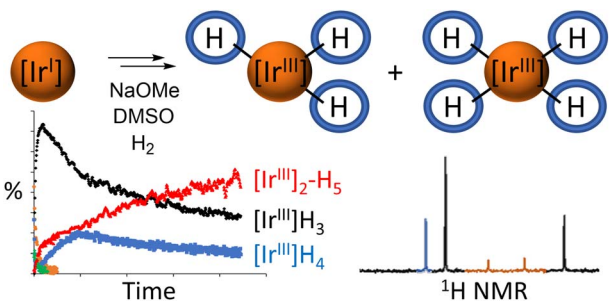
Surusch Djalali, Yun Jing, Yu Ogawa* and Martina Delbianco*



1396

Iridium trihydride and tetrahydride complexes and their role in catalytic polarisation transfer from *para*hydrogen to pyruvate

Ben. J. Tickner and Simon B. Duckett*



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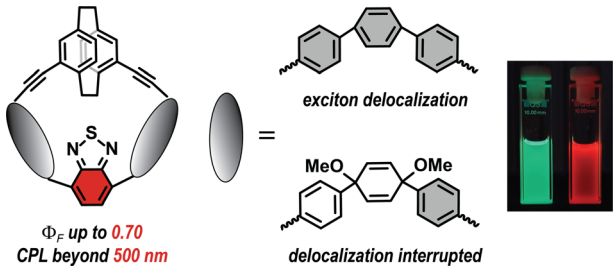
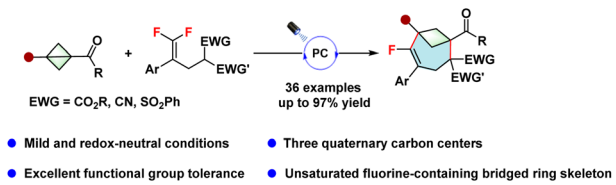
1405



Role of exciton delocalization in chiroptical properties of benzothiadiazole carbon nanohoops

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

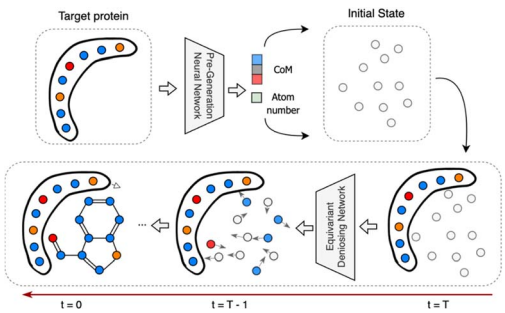
1411



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*

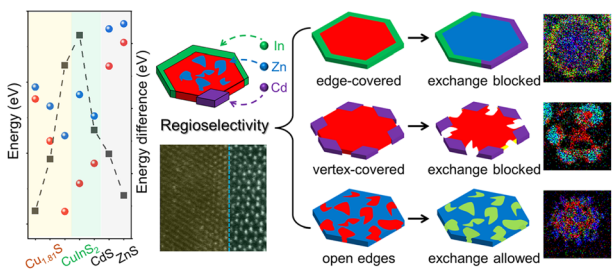
1417



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*

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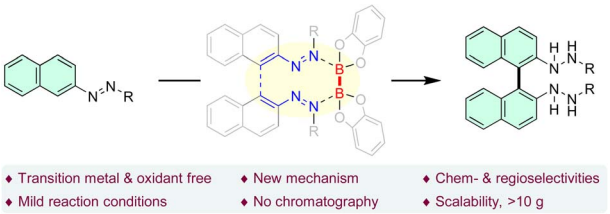
1441

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

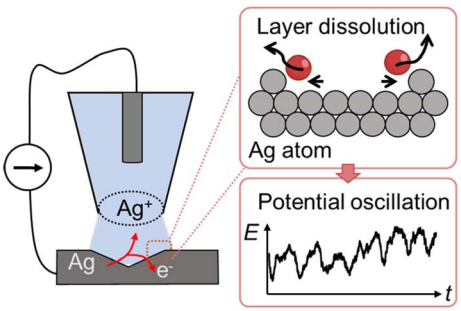
Liang-Wen Qi, Emmanuella Bema Twumasi, Xiao-Wei Li, Rui Li and Yixin Lu*



1447

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

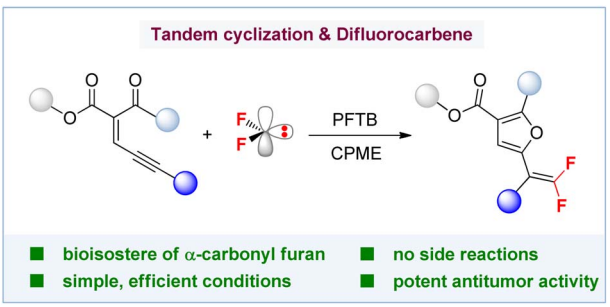
Yufei Wang, Roberto Garcia-Carrillo and Hang Ren*



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*

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