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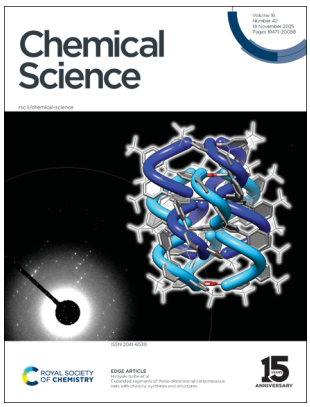
IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 16(42) 19471–20088 (2025)



Cover
See Hiroyuki Isobe *et al.*, pp. 19594–19600. Image reproduced by permission of Hiroyuki Isobe from *Chem. Sci.*, 2025, **16**, 19594.

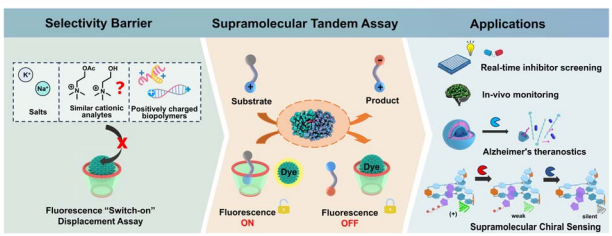
Inside cover
See Shun Dekura, Motohiro Mizuno and Hatsumi Mori, pp. 19601–19607. Image reproduced by permission of Shun Dekura, Motohiro Mizuno and Hatsumi Mori from *Chem. Sci.*, 2025, **16**, 19601. The artwork was designed by ART ACTION Inc., Japan.

COMMENTARY

19489

A reflection on enzyme-coupled supramolecular sensing: overcoming selectivity barriers with macrocyclic reporter pairs

Shuangqi Song and Yu Liu*

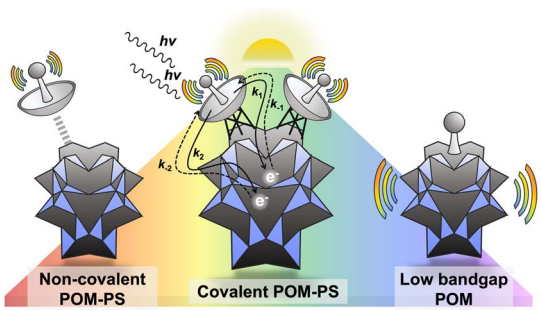


PERSPECTIVES

19493

Unveiling photoinduced electron transfers in photosensitized polyoxometalates for solar energy conversion

Christian Cariño, Anna Proust, Geoffroy Guillemot, Ludivine K/Bidi, Sébastien Blanchard, Elizabeth A. Gibson and Guillaume Izzet*



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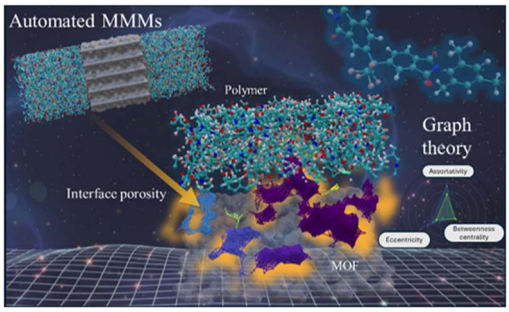
PERSPECTIVES

19519

MOF surface morphology governs interfacial pore architecture and CO_2 dynamics in mixed matrix membranes

Alejandro Diaz-Marquez, Supriyo Naskar, Dong Fan, Mohamed Eddaoudi and Guillaume Maurin*

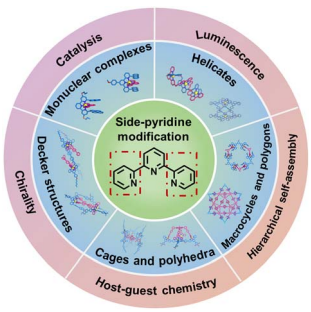


REVIEWS

19532

Novel metallo-supramolecular architectures based on side-pyridine-modified terpyridines: design, self-assembly, and properties

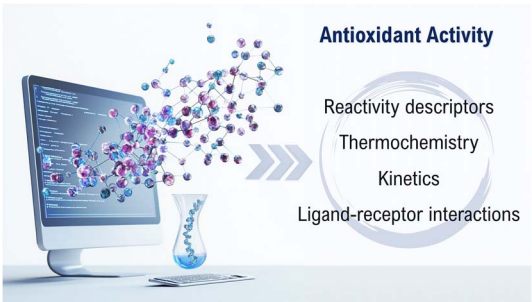
Ningxu Han, Xin Jiang* and Ming Wang*



19570

Antioxidant activity at the molecular level: exploring ways of action and computational tools to investigate them

Annia Galano*

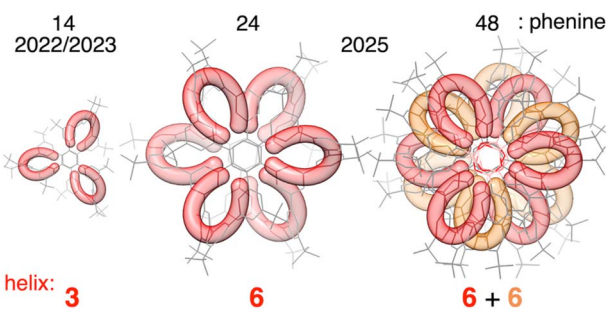


EDGE ARTICLES

19594

Expanded segments of three-dimensional carbonaceous nets with chirality: synthesis and structures

Toshiya M. Fukunaga, Kiyofumi Takaba, Satoshi Yoshida, Saori Maki-Yonekura, Koji Yonekura and Hiroyuki Isobe*



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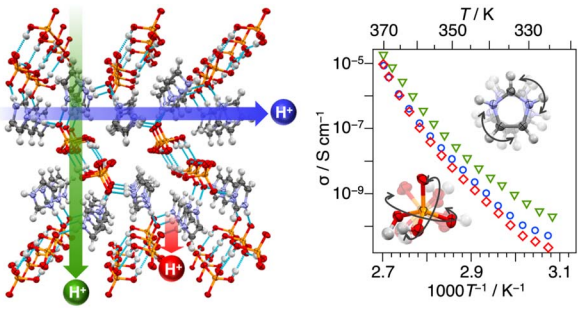
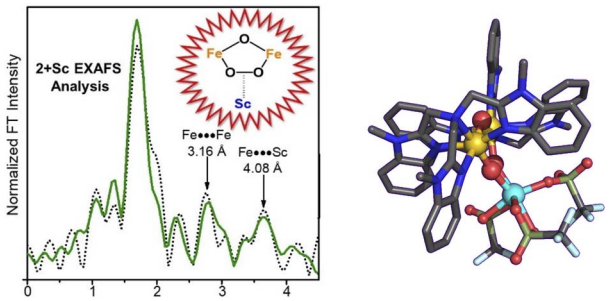


Isotropic proton conduction in an anisotropic crystal: the role of molecular rotational dynamics in imidazolium dihydrogen phosphate

Shun Dekura,* Motohiro Mizuno and Hatsumi Mori*

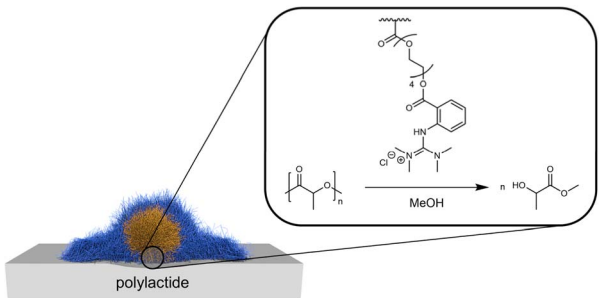
19608



Mimicking sMMOH chemistry: trapping the Sc^{3+}-bound nonheme Fe^{III}–O–O–Fe^{III} adduct prior to its conversion into an $Fe^{IV}_2(\mu\text{-}O)_2$ core

Patrick M. Crossland, Bittu Chandra, Saikat Banerjee, Chase S. Abelson, Yisong Guo,* Marcel Swart* and Lawrence Que*

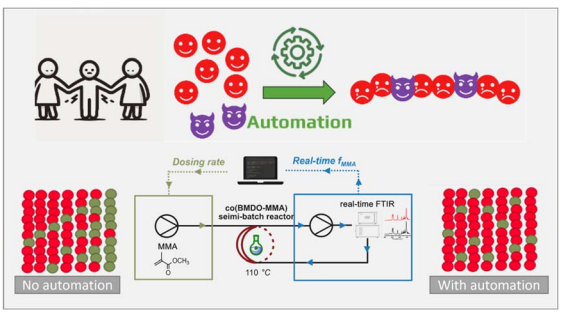
19614



Depolymerization of PLA catalyzed by guanidine-modified microgels

Fabian Fink, Frédéric Grabowski, Sandra Oden, Paul Nisgutski, Andrij Pich* and Sonja Herres-Pawlis*

19624



Synthesis of biodegradable vinyl copolymers *via* enforced regular sequence distribution from automated radical ring opening polymerisation

Mengyuan Wen, WeiNian Wong and Tanja Junkers*

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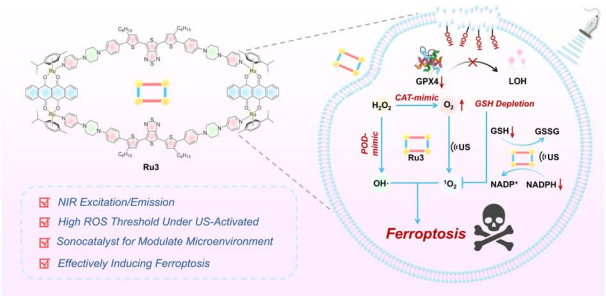
19632

Rationally designed sonocatalyst-enhanced supramolecular ferroptosis inducers for effective cancer therapy

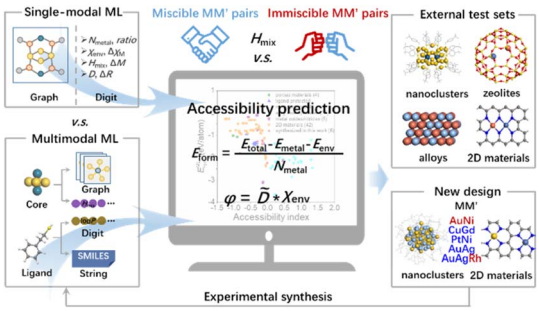
Yida Pang, Yong Luo, Ting Liu, Qian Li, Longcan Mei, Junhua Zhang, Chonglu Li,* Junrong Li* and Yao Sun*



19644

High-throughput design of bimetallic materials *via* multimodal machine learning and the accessibility index

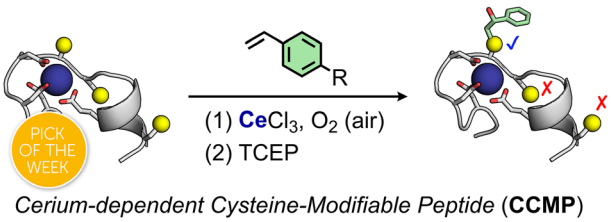
Yuming Gu, Yating Gu, Maochen Yang, Shisi Tang, Jiawei Chen, Xinyi Liang, Dong Zheng, Zekun Li, Fengqi Song, Yang Gao, Yan Zhu,* Yinghuan Shi* and Jing Ma*



19658

Cerium-mediated site-selective cysteine functionalization

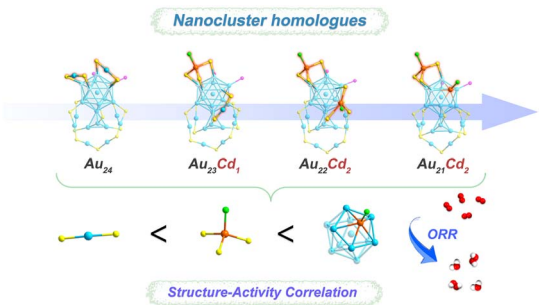
Jaewon Lee and Woon Ju Song*



19669

Construction of a homologous series of metal nanoclusters and implications for structure–activity correlations

Qinzhen Li, Tingting Jiang, Sha Yang, Jinsong Chai,* Haizhu Yu* and Manzhou Zhu*



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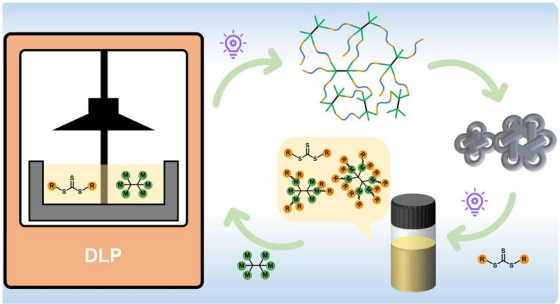
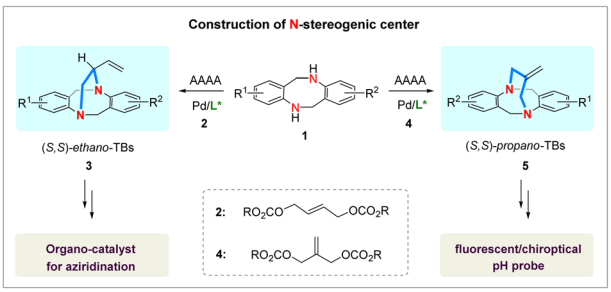


Recyclable RAFT-3D printing

Xiaofeng Pan, Xinggang Luo, Xiangqiang Pan, Jiajia Li* and Jian Zhu*

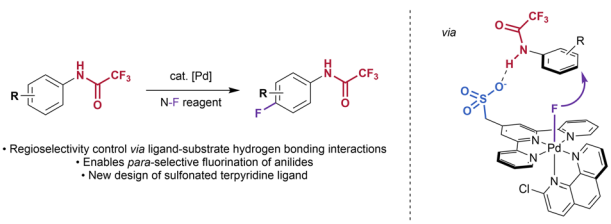
19683



Catalytic enantioselective construction of two N-stereogenic centers of *ethano*- and *propano*-Tröger's bases

Chun-Yan Guan, Tao Lu, Ya Li, Chao-Hua Liu, Xiao Xiao and Guang-Jian Mei*

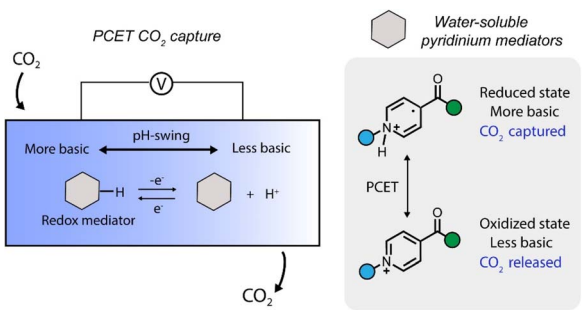
19694



The development of sulfonated terpyridine ligands for control of regioselectivity in palladium-catalysed fluorination of anilides

Jiri Dolezel and Robert J. Phipps*

19702



Water-soluble pyridinium redox mediators for pH-swing CO_2 capture

Eloi Grignon, Zhangfei Su, Jiang Tian Liu, Armanda Lima, Andrew Wang, Parisa Karimi, Shuai Chen* and Dwight S. Seferos*

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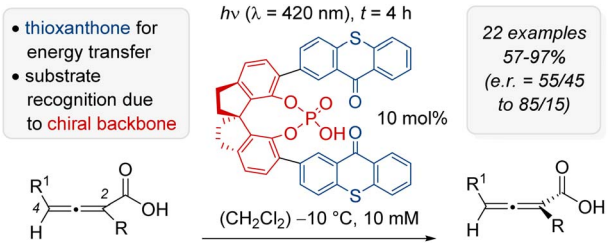
19711

Photochemical deracemization of 2,3-allenoic acids mediated by a sensitizing chiral phosphoric acid catalyst

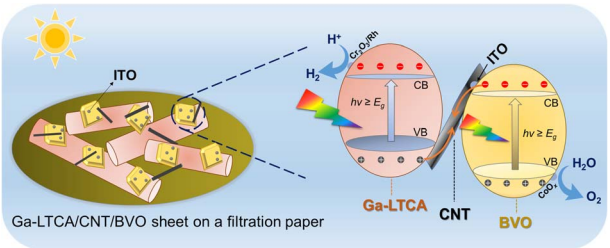
Max Stierle, Daniel Bitterlich, Julia Westermayr and Thorsten Bach*



19720

Z-scheme overall water splitting on photocatalyst sheet mediated by carbon nanotubes using oxysulfide photocatalyst responsive to long wavelengths

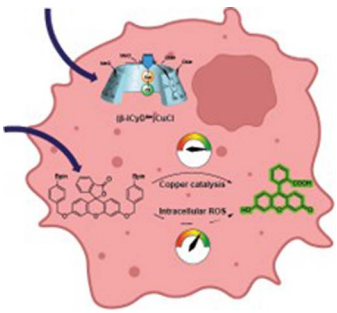
Long Wang, Chen Gu, Tsuyoshi Takata, Nobuyuki Zettsu, Swapnil S. Karade, Swarnava Nandy, Joji Yoshimura, Yasutaka Nishi, Kiyoshi Kanie, Takashi Hisatomi and Kazunari Domen*



19727

Encapsulating NHC–capped copper(I) complexes inside cyclodextrin for catalysis in living cells

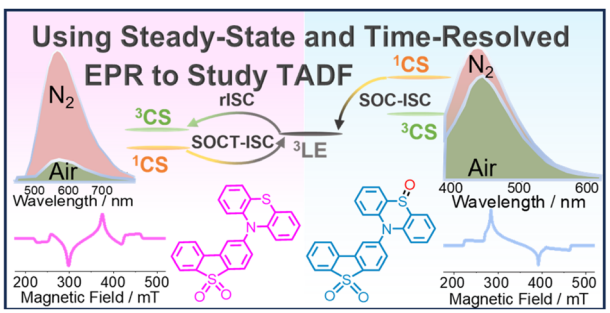
Francisca Figueiredo, Hugo Madec, Pierre Mesdom, Giulia Salluce, Yanis Tigherghar, Kevin Cariou,* Sylvain Roland,* Matthieu Sollogoub* and Gilles Gasser*



19737

Study of the thermally-activated delayed fluorescence (TADF) mechanism of phenothiazine–dibenzothiophene-*S*,*S*-dioxide electron donor–acceptor dyads using steady-state and time-resolved optical and electron paramagnetic resonance spectroscopies

Yuying Pei, Andrey A. Sukhanov, Xi Chen, Greta Sambucari, Laura Bussotti, Xin Liu, Jianzhang Zhao,* Yanqin Li,* Yanping Huo,* Violeta K. Voronkova,* Huimin Guo* and Mariangela Di Donato*



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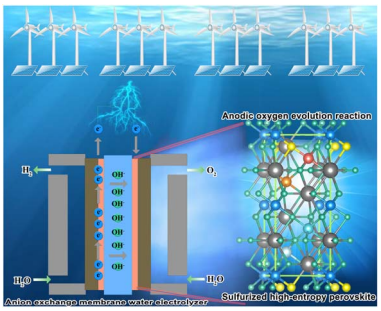
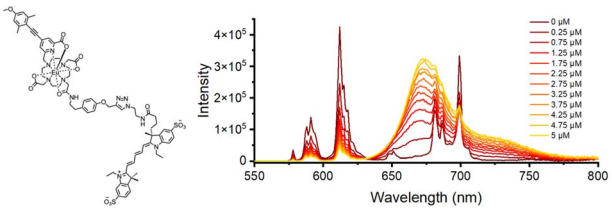


Regulating metal–oxygen covalency in reconstructed sulfurized high-entropy perovskite to activate and stabilize lattice oxygen for the oxygen evolution reaction

Xiang Li, Qiuju Li, Bingyu Chen, Mengna Wang, Chuanchuan Yan, Subhajit Jana, Ziqi Liao, Zhenyu Li,* Dunfeng Gao and Guoxiong Wang*

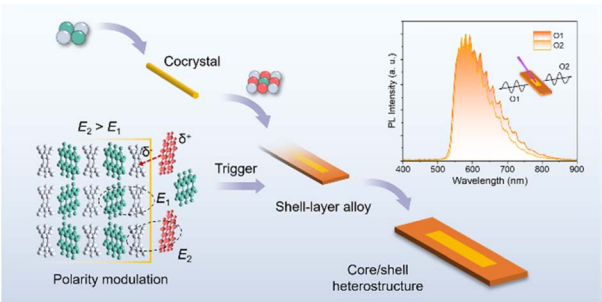
19762



Temperature dependent luminescence of europium/cyanine FRET pairs

Tsz Lam Cheung and David Parker

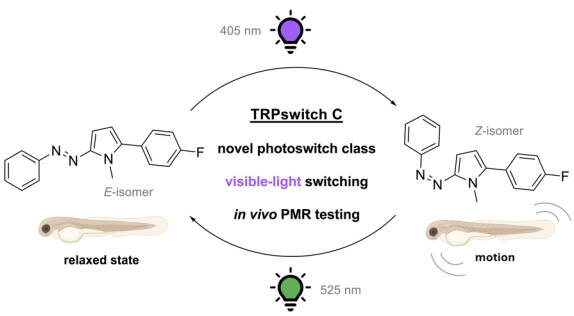
19769



Interfacial polarity-driven self-assembly of organic core/shell heterostructures with directional Fabry–Pérot resonance

Jin Feng, Zhen-Yu Geng, Yi Zong, Chuan-Zeng Wang, Shu-Hai Chen, Hong-Tao Lin,* Li-Wei Xie* and Xue-Dong Wang*

19777



Aryl azopyrroles as visible light photoswitchable TRPA1 ligands

Lisa C. Dollhopf, Jordan A. Munos, Kai Y. Zheng, Rui Xin Tao, Peter R. Haycock, Philip J. Parsons, Randall T. Peterson, Pui-Ying Lam* and Matthew J. Fuchter*

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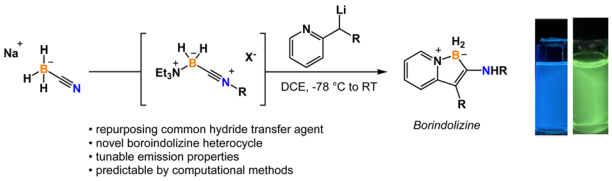
19786

A borindolizine platform for the design of fluorophores with tunable emissions

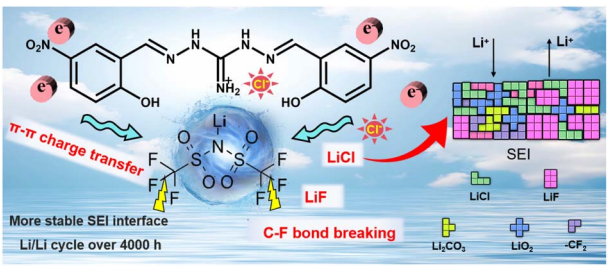
Chirag N. Apte, Nicholas W. Heller, Ben Zhen Huang, Adam Marr, Kjell Jorner, Alan Aspuru-Guzik and Andrei K. Yudin*



19792

Tailoring the electronic structure to enable rapid Li-ion diffusion and a stabilized LiF–LiCl rich electrode–electrolyte interface

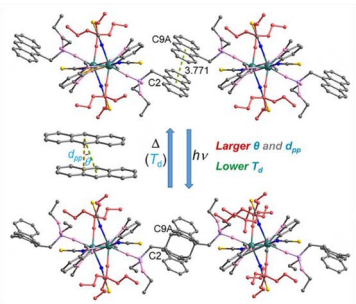
Shan Su, Xuanyi Zhou, Weizhong Liang, Zhuoriu Su, Yibing Qu, Yuhan Zhong, Jinghong Qiu and Biao Zhang*



19806

Photoresponsive luminescent single-molecule magnets based on dysprosium–anthracene complexes: regulating the de-dimerization temperature of the photocycloaddition product by co-ligand

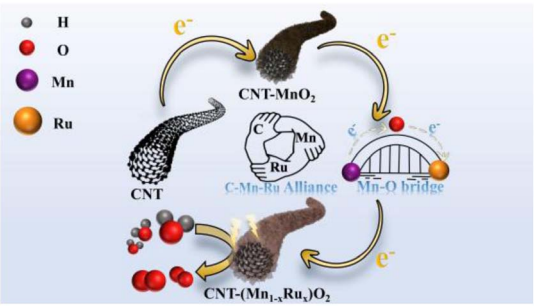
Ye-Hui Qin, Xiu-Fang Ma, Xinlan Hou, Xin-Da Huang, Song-Song Bao, Yuxi Tian, Yi-Quan Zhang* and Li-Min Zheng*



19820

Structurally engineered CNT-confined $Mn_xRu_{1-x}O_2$ catalysts for efficient acidic oxygen evolution at low Ru loading

Xiaolin Zheng, Xiaofei Miao, Zijie Yang, Zhaoyan Luo, Jun Yu, Huiqi Li* and Lei Zhang*



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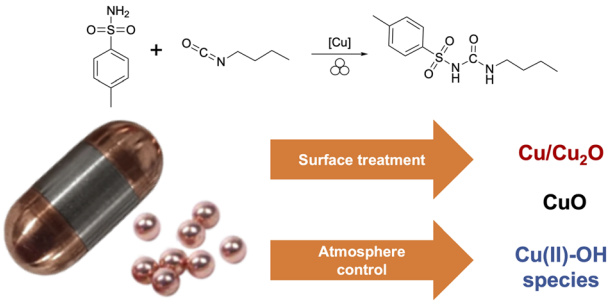
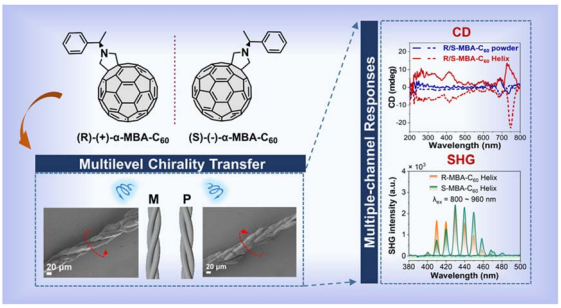
19830



Harnessing the copper surface for direct mechanocatalysis: a case study on mechanochemical sulfonylurea synthesis

Kathleen R. Floyd, Lizette S. Mella, Ryan W. Kwok, Mackenzie Gray, Edward J. Broker, Jr., Mateusz Marianski, Tomislav Friščić and James D. Batteas*

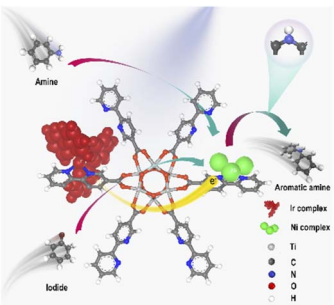
19843



Multilevel chirality transfer and second harmonic generation in mesoscopic double helical supramolecular self-assemblies of fullerene enantiomers

Jinrui Li, Kaipeng Zhuang, Yunlong Tao, Qingfeng Zhang,* Hongguang Li* and Jingcheng Hao

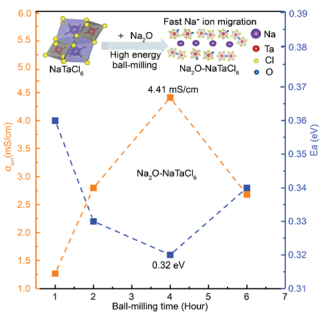
19849



Dual-catalytic architectures accommodated by titanium-oxo clusters boosting visible-light-driven C–N cross-coupling *via* intramolecular electron transfer

Shiyu Wang, Jianfeng Jia, Yongqi Wang, Qiang Gao* and Gang Ye*

19857



Break it down to speed it up: Na_2O–$NaTaCl_6$

Islamiyat A. Ojelade, Erica Truong, Ifeoluwa P. Oyekunle, Tej P. Poudel, Yudan Chen, Michael J. Deck, Yongkang Jin, Bright Ogbolu, Pawan K. Ojha, Md. Mahinur Islam, Thilina N. D. D. Gamaralalage, J. S. Raaj Vellore Winfred and Yan-Yan Hu*

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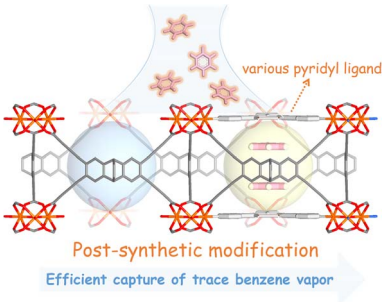
19867

Efficient capture of trace benzene vapor by metal–organic frameworks modified with macrocyclic pyridyl ligands

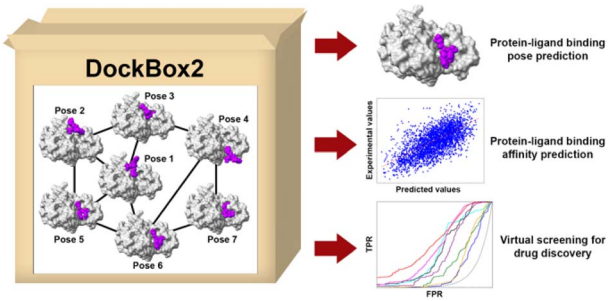
Gang Liang, De-Jian Chen, Zhu-Jun Long, Hao Zhuo, Xiao-Feng Zhong, Xiong-Hai Chen, Huai-Yu Shao, Zong-Wen Mo* and Xiao-Ming Chen



19876

Pose ensemble graph neural networks to improve docking performances

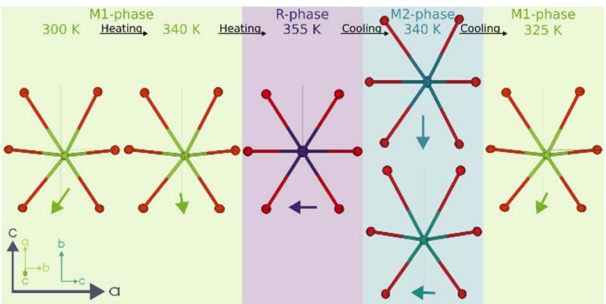
Thanawat Thaingtamtanha, Jordane Preto and Francesco Gentile*



19888

Single-crystal synchrotron X-ray diffraction study reveals bulk intermediate M2 phase during the VO_2 insulator-to-metal transition

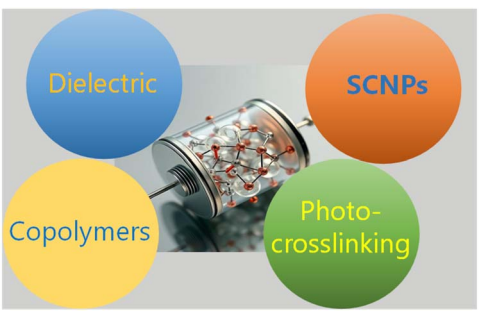
Jacob Svane, Michael Anthony Quintero, Emilie Skytte Vosegaard, Magnus Kløve, Daniel Alexander Mayoh, Geetha Balakrishnan and Bo Brummerstedt Iversen*



19898

Anthracene-functionalized dipolar glass copolymers as precursors for high-dielectric single-chain nanoparticles

Sebastian Bonardd,* Jon Maiz, Javier Maisueche, Ester Verde-Sesto and José A. Pomposo*



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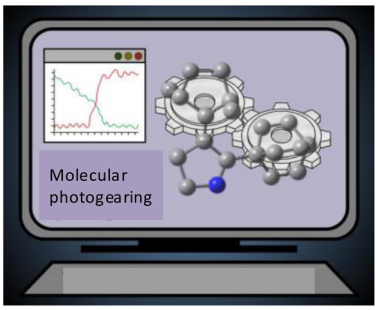
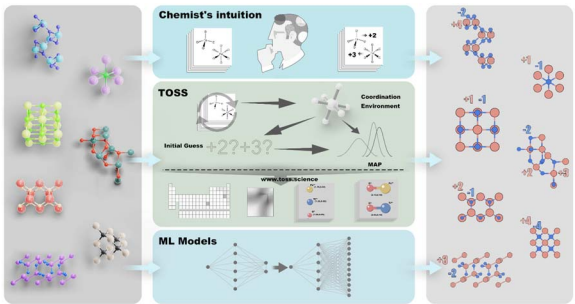
19910



Achieving one-step molecular photogearing in a minimal light-driven molecular motor

Enrique M. Arpa* and Bo Durbeej*

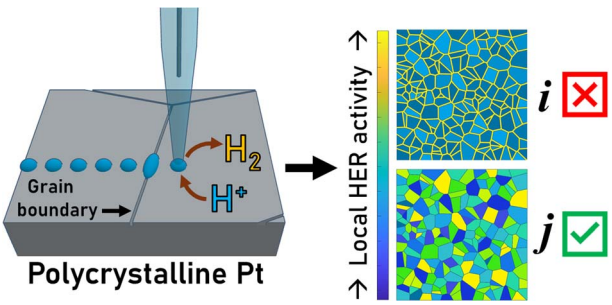
19917



Oxidation states in solids from data-driven paradigms

Yue Yin and Hai Xiao*

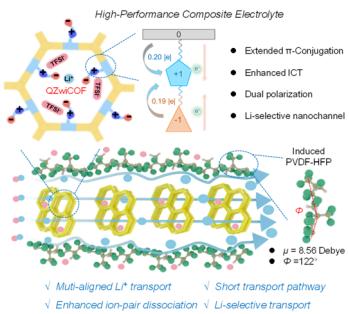
19929



Intrinsic electrocatalytic activity of platinum grain boundaries: correcting measurement artefacts in scanning electrochemical cell microscopy (SECCM)

Harry B. Swan, Lachlan F. Gaudin, Alannah J. Hunt and Cameron L. Bentley*

19944



Dual polarization in extended π-conjugated zwitterionic COF facilitates Li^+ aligned transportation for high-performance solid-state lithium–metal batteries

Linchu Xu, Feng Chen, Ju Duan, Kexiang Wang, Jiaqiang Li, Jingzhao Wang, Jianan Wang, Wei Lyu* and Yaozu Liao*

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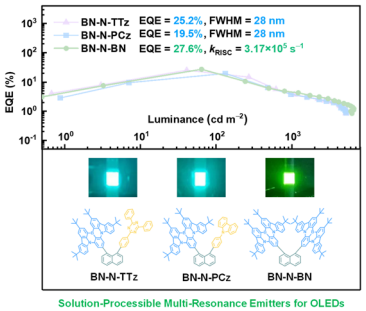
19956

Enhancing the reverse intersystem crossing (RISC) rates and efficiencies of MR-TADF emitters with a U-shaped molecular structure for solution-processed OLEDs

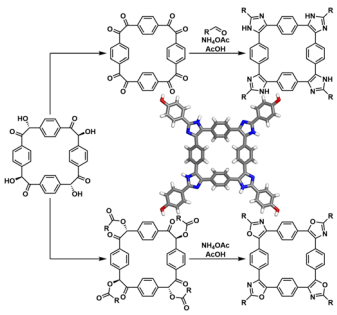
Shipan Xu, Wenping Liu, An Yan, Xuyang Du, Yuanhui Sun,* Junfei Tao, Guijiang Zhou,* Zhao Chen* and Xiaolong Yang*



19967

Inverted azolophanes: alternant *o*-heteroarene/*p*-arene macrocycles

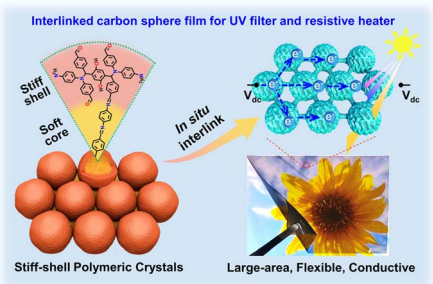
Yun-Hsien Lin, Xiqu Wang, Dariusz W. Szczepanik,* Paweł A. Wieczorkiewicz and Ognjen Š. Miljanić*



19973

Large-area, flexible, and conductive porous films of interlinked carbon nanospheres for UV light filters and resistive heaters

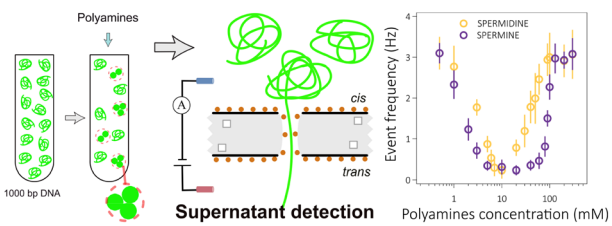
Meng-Qi Zhao, Tian-Yi Li, Chuan-Bin Li, Hui-Qun Huang, Yong-Sheng Wang, Ling-Yu Dong, Xiao-Dong Shi, Yu-Tai Wu, Guang-Ping Hao* and An-Hui Lu*



19981

DNA aggregation and resolubilization in the presence of polyamines probed at the single molecule level using nanopores

Yuhua Cai, Benjamin Cressiot, Sébastien Balme, Eric Raspaud, Laurent Bacri* and Juan Pelta*



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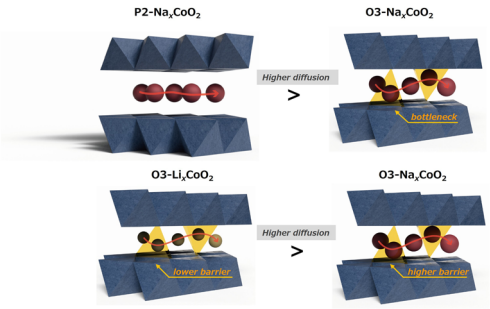
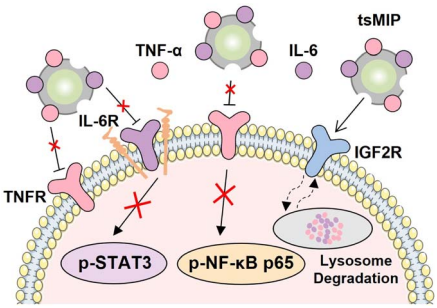
19990



Revisiting the ion dynamics in Li_xCoO_2 and Na_xCoO_2

Ryoichi Tatara,* Daisuke Igarashi, Masanobu Nakayama, Tomooki Hosaka, Kazuki Ohishi, Izumi Umegaki, Jumpei G. Nakamura, Akihiro Koda, Hiroto Ohta, Rasmus Palm, Martin Månsson, Eun Jeong Kim, Kei Kubota, Jun Sugiyama and Shinichi Komaba*

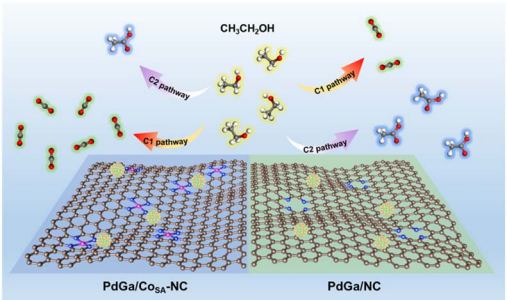
20002



Tri-specific molecularly imprinted lysosomal nanodegrader enables synergistic therapy of cytokine storm

Jingran Chen, Weihua Lu, Ying Li, Zhanchen Guo, Qian Liu, Weiwei Liu, Lisheng Wang and Zhen Liu*

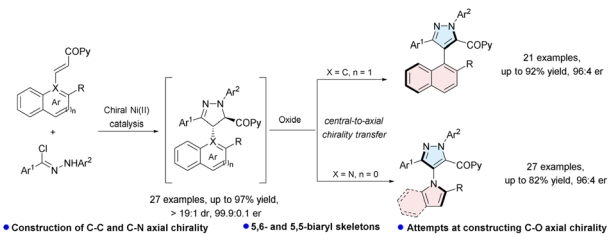
20012



PdGa nanoalloys loaded on single atom Co dispersed nitrogen doped carbon for ethanol electrooxidation: improved C1 pathway selectivity and durability

Chengming Huang, Xia Chen, Wenjing Zhang, Fangzheng Wang, Yunchuan Tu,* Jing Li* and Zidong Wei*

20021



Enantioselective synthesis of C–C and C–N axially chiral pyrazole-based heterobiaryls

Jun He, Zun Yang, Lili Lin* and Xiaoming Feng*

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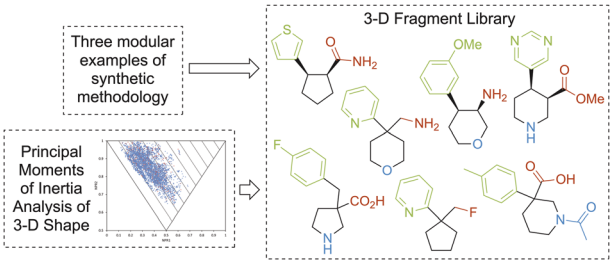
20030

Design, modular synthesis and screening of 58 shape-diverse 3-D fragments

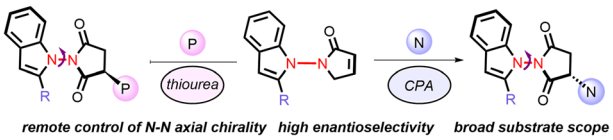
Thomas D. Downes, S. Paul Jones, James D. Firth, John F. Darby, Amelia K. Gilio, Hanna F. Klein, Xinyu Wang, David C. Blakemore, Claudia De Fusco, Stephen D. Roughley, Lewis R. Vidler, Maria Ann Whatton, Alison J.-A. Woolford, Gail L. Wrigley, Roderick E. Hubbard, Liang Wu, Gideon J. Davies and Peter O'Brien*



20042

Remote generation of N–N axial chirality through asymmetric hydrophosphinylation/hydroamination of maleimides

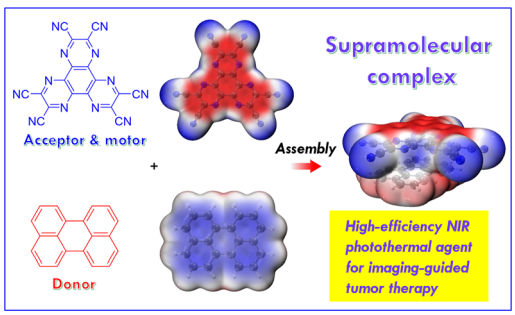
Yu-Li Sun, Lei Dai, Kun Zhu, Qingqin Huang, Yushuang Chen, Zugen Wu and Yixin Lu*



20048

An acceptor motor-driven electronic donor–acceptor supramolecular scaffold towards imaging-guided tumor therapy

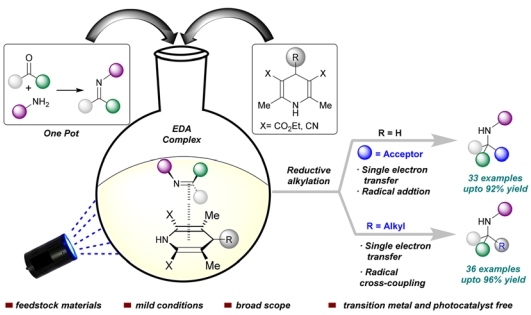
Canze Zheng, Liwei Zhu, Jianyu Zhang, Xin Deng, Zhengyao Zhong, Xiang He, Qiaoyun Zhang, Junkai Liu, Miao Meng, Jacky W. Y. Lam, Ying Li,* Ming Chen* and Ben Zhong Tang*



20061

Electron donor–acceptor complex offers a diverse approach for carbonyl alkylative amination

Hrishikesh Paul, Arijit Chakraborty, Animesh Mandal, Dibyangshu Das, Sanat Kumar Mahapatra, Lisa Roy* and Indranil Chatterjee*



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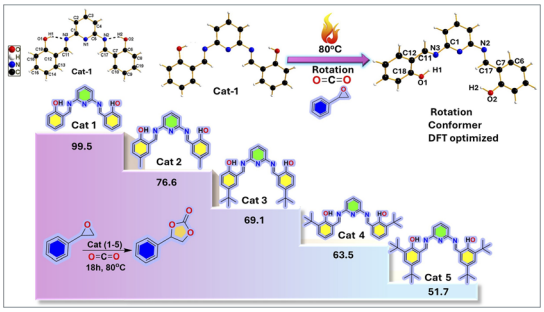

Thermally driven conformational tuning of pyridine bis-salicylaldimine for efficient CO_2 activation and cyclic carbonate formation under mild conditions

Veenu Mishra, Siddhi Kediya, Devender Goud, Diku Raj Deka, Subhajit Chakraborty and Sebastian C. Peter*

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