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IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 16(20) 8597–9032 (2025)

Cover
See Dominik Stemer, Stephan Thürmer, Bernd Winter *et al.*, pp. 8637–8647. Image reproduced by permission of Dominik Stemer from *Chem. Sci.*, 2025, **16**, 8637. The authors would like to thank Vanessa Shababzadeh for the design and production of the cover illustration.

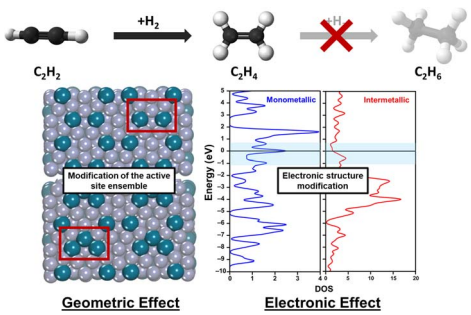
Inside cover
See Haibo Xie *et al.*, pp. 8648–8660. Image reproduced by permission of Haibo Xie from *Chem. Sci.*, 2025, **16**, 8648.

REVIEW

8611

Structural chemistry of intermetallic compounds for active site design in heterogeneous catalysis

Nilanjan Roy, Kathryn MacIntosh, Mustafa Eid, Griffin Canning and Robert M. Rioux*

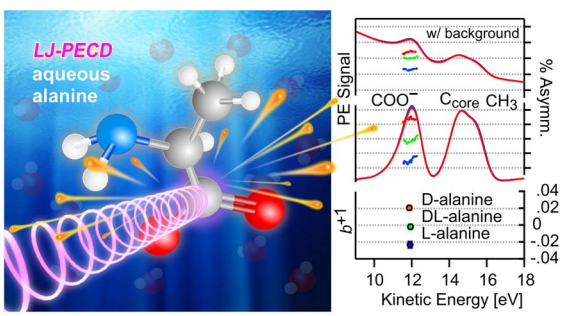


EDGE ARTICLES

8637

Photoelectron circular dichroism of aqueous-phase alanine

Dominik Stemer,* Stephan Thürmer,* Florian Trinter, Uwe Hergenhahn, Michele Pugini, Bruno Credidio, Sebastian Malerz, Iain Wilkinson, Laurent Nahon, Gerard Meijer, Ivan Powis and Bernd Winter*



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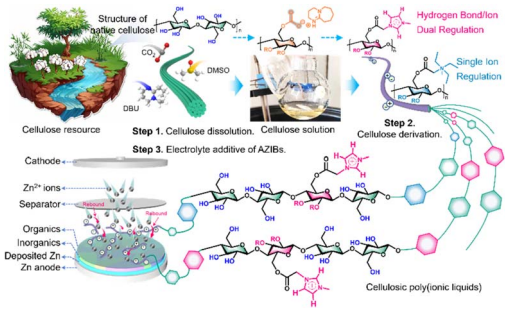
EDGE ARTICLES

8648

Design of cellulosic poly(ionic liquid)s with a hydrogen bond/ion dual regulation mechanism for highly reversible Zn anodes

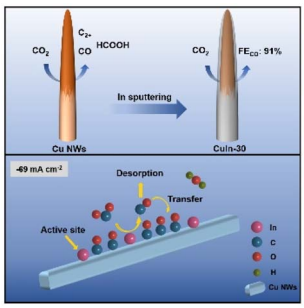
Kui Chen, Yongzhen Xu, Hebang Li, Yue Li, Lihua Zhang, Yuanlong Guo, Qinqin Xu, Yunqi Li and Haibo Xie*



8661

Tuning intermediate binding enables selective electroreduction of carbon dioxide to carbon monoxide on a copper–indium catalyst

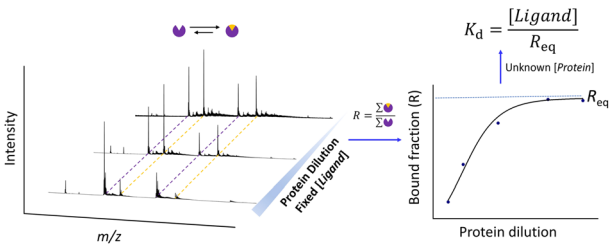
Shengzhou Xu, Chenglong Wang, Chunjing Ran, Hexing Yang, Wangjiang Gao, Bitao Dong,* Yuhang Liu and Dan Ren*



8673

A straightforward method for measuring binding affinities of ligands to proteins of unknown concentration in biological tissues

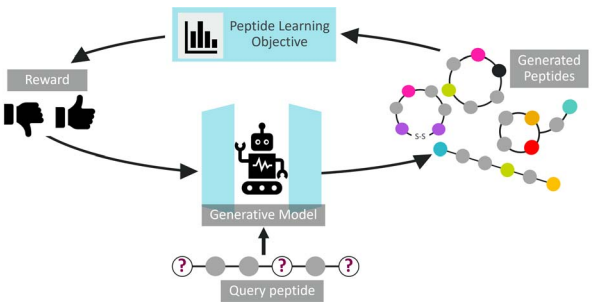
Bin Yan* and Josephine Bunch*



8682

PepINVENT: generative peptide design beyond natural amino acids

Gökçe Geylan,* Jon Paul Janet, Alessandro Tibo, Jiazhen He, Atanas Patronov, Mikhail Kabeshov, Werngard Czechtizky, Florian David, Ola Engkvist and Leonardo De Maria



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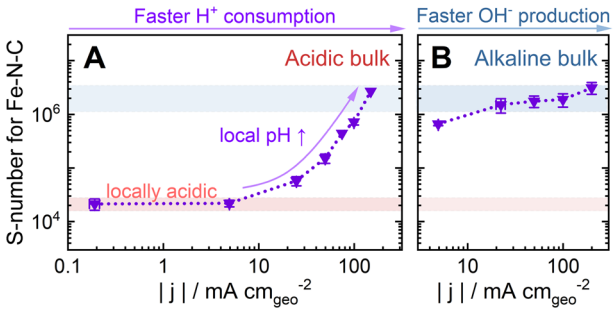
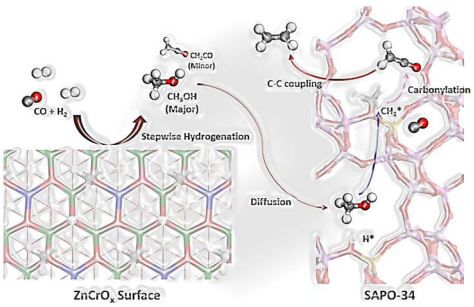


Establishing the stability number descriptor for Fe–N–C fuel cell electrocatalysts

Yu-Ping Ku,* Kavita Kumar, Antoine Bonnefont, Li Jiao, Marco Mazzucato, Christian Durante, Frédéric Jaouen and Serhiy Cherevko*

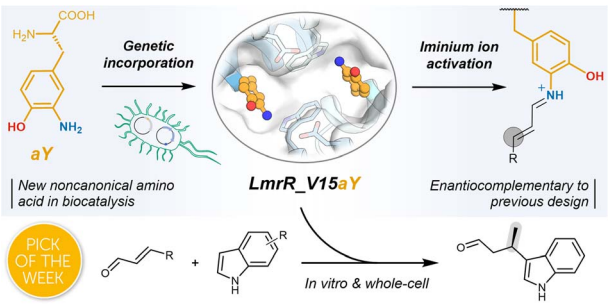
8711



Unraveling the mechanisms of ketene generation and transformation in syngas-to-olefin conversion over $ZnCrO_x$|SAPO-34 catalysts

Zhuo-Yan Yao, Sicong Ma* and Zhi-Pan Liu*

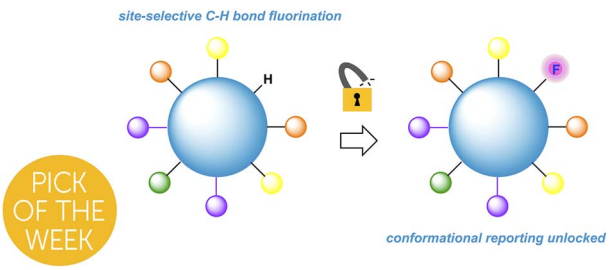
8721



Genetically encoded 3-aminotyrosine as catalytic residue in a designer Friedel–Crafts alkylase

Bart Brouwer, Franco Della-Felice, Andy-Mark W. H. Thunnissen and Gerard Roelfes*

8729



A highly selective C–H bond fluorination unlocks conformational reporting in a complex natural product derivative

Jonah Ruskin, Roxanne Dekeyser, Nathaniel Garrison, Phoebe Williams, Maya Kramer-Johansen, Ananya Majumdar, Travis Dudding,* Adam Huczyński* and Thomas Lectka*

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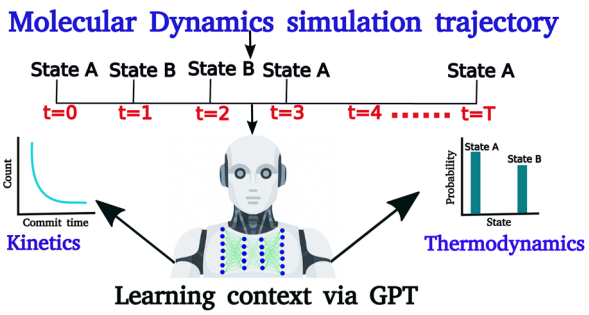
Accurate prediction of the kinetic sequence of physicochemical states using generative artificial intelligence

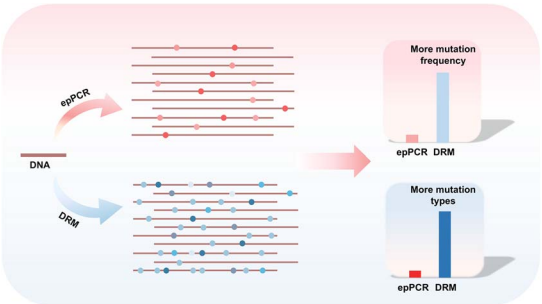
Palash Bera* and Jagannath Mondal*



8752

Deaminase-driven random mutation enables efficient DNA mutagenesis for protein evolution

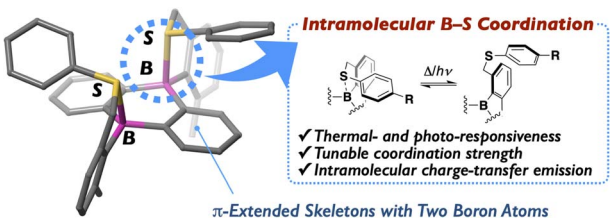
Ying Hao, Tong-Tong Ji, Shu-Yi Gu, Shan Zhang, Yao-Hua Gu, Xia Guo, Li Zeng, Fang-Yin Gang, Jun Xiong, Yu-Qi Feng,* Neng-Bin Xie* and Bi-Feng Yuan*



8764

Intramolecular arylsulfide-coordinated diboraanthracenes: effect of B–S coordination on ground-state and excited-state behavior

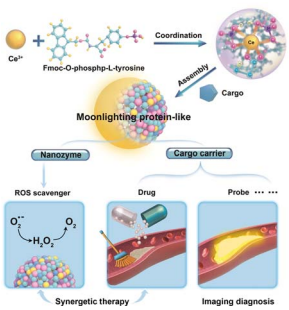
Hiroki Narita, Alexander Virovets, Hans-Wolfram Lerner, Matthias Wagner and Shigehiro Yamaguchi*



8772

Multifunctional cerium-based nanozymes as moonlighting protein mimics for atherosclerosis diagnosis and therapy

Gui-Mei Han, Jing-Qi Liu, Zhi-Qi Dai, Wei-Liang Jin, Qi-Liang Cai,* De-Ming Kong* and Li-Na Zhu*



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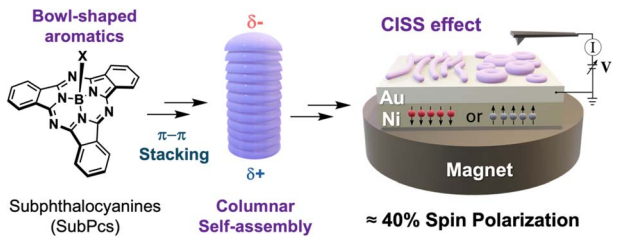
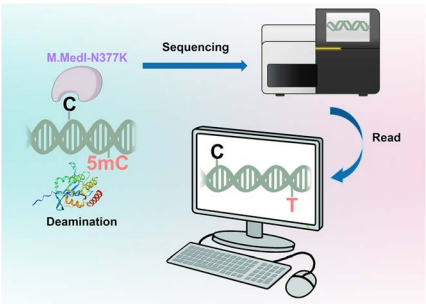


Spin filtering in self-assembled bowl-shaped aromatics

Jorge Labella,* Anu Gupta, Anil Kumar, Elisa López-Serrano, Deb Kumar Bhowmick, Ron Naaman* and Tomás Torres*

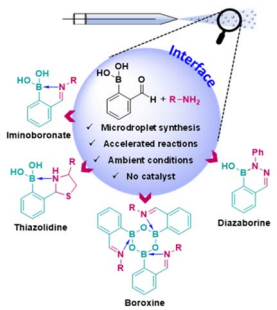
8788



Direct single-nucleotide resolution sequencing of DNA 5-methylcytosine using engineered DNA methyltransferase-mediated CMD-seq

Wei Liu, Zhao-Cheng Ma, Shan Zhang, Fang-Yin Gang, Tong-Tong Ji, Yao-Hua Gu, Neng-Bin Xie, Shu-Yi Gu, Xia Guo, Tian Feng, Yu Liu,* Jun Xiong* and Bi-Feng Yuan*

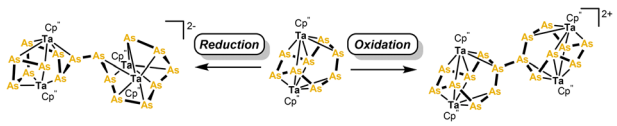
8800



Accelerated click reactions using boronic acids for heterocyclic synthesis in microdroplets

Jyotirmoy Ghosh and R. Graham Cooks*

8807



Redox mediated dimerisation of a *cyclo*-As_8 complex

Christoph Riesinger and Manfred Scheer*

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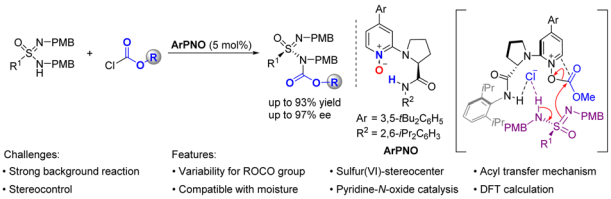
Pyridine-*N*-oxide catalyzed asymmetric *N*-acylative desymmetrization of sulfonimidamides

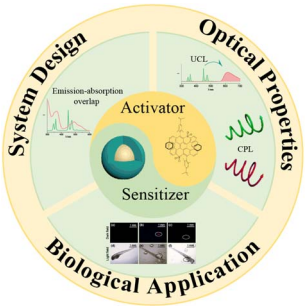
Cui-Mei Guo, Fang-Yuan Zhang, Yin Tian,* Ming-Sheng Xie* and Hai-Ming Guo*



8820

Boosting near-infrared-triggered photon upconversion in optical nanomaterials *via* lanthanide-doped nanoparticle sensitization

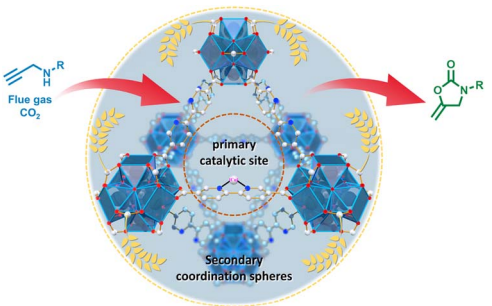
Jiangshan Luo, Junjian Shen, Xingwen Cheng,* Yan Liu, Xiulian Yin, Tianxi Hu, Guangxin Fan, Jianming Zhang, Wei Zheng* and Xueyuan Chen*



8827

Tailored engineering of primary catalytic sites and secondary coordination spheres in metalloenzyme-mimetic MOF catalysts for boosting efficient CO_2 conversion

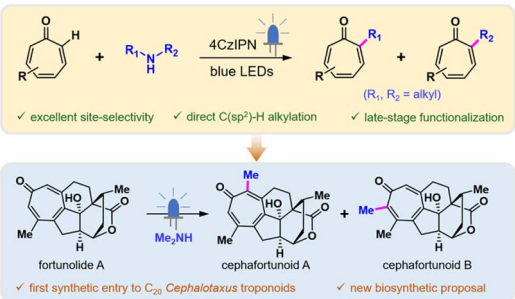
Jiawei Li,* Fan Yang, Benling Yu, Zhongke Dai, Shiyuan Wei, Ying Wu,* Liuqing He, Fa Zhou, Jianhan Huang* and You-Nian Liu



8836

Visible-light-mediated site-selective C(sp^2)–H alkylation of tropones facilitates semi-synthesis of cephafortunoids A and B

Qi-Xiang Zeng, Cheng-Yu Zheng, Zhan-Peng Ge, Jin-Xin Zhao* and Jian-Min Yue*



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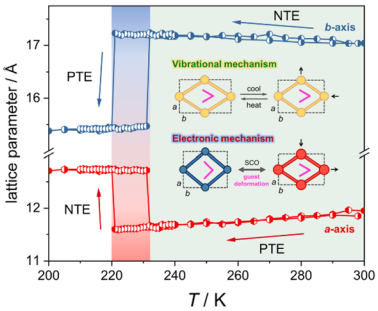
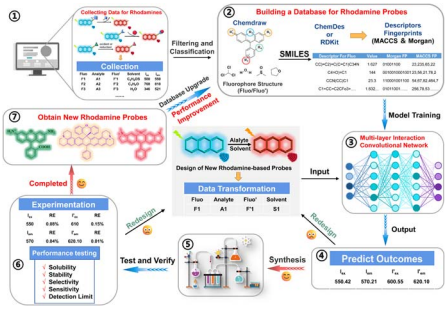


Switchable colossal anisotropic thermal expansion in a spin crossover framework

Si-Guo Wu, Wen Cui, Ze-Yu Ruan, Zhao-Ping Ni* and Ming-Liang Tong*

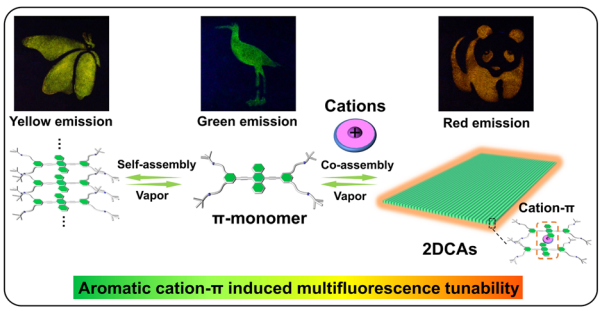
8853



Enhancing fluorescent probe design through multilayer interaction convolutional networks: advancing biosensing and bioimaging precision

Gongcheng Ma, Qihang Ding,* Yuding Zhang, Xiaodong Zeng, Kai Zhu, Hongli Chen, Wenxuan Zhang, Qingzhi Wang, Shuman Huang, Ping Gong,* Zhengwei Xu* and Xuechuan Hong*

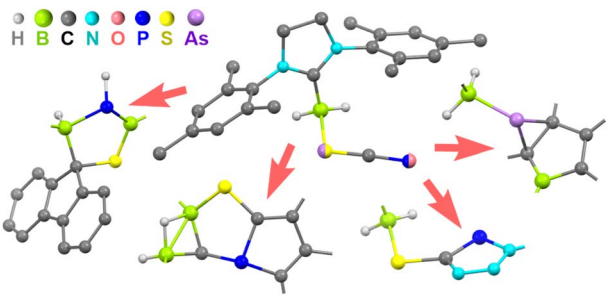
8861



Aromatic cation–π induced multifluorescence tunable two-dimensional co-assemblies for encoded information security

Zhao Gao, Jianxiang Sun, Lulu Shi, Wei Yuan and Wei Tian*

8870



Synthesis and reactivity of a parent phosphathioethynolato-borane and a boraarsaketene

Malte Jürgensen, Tanja Kunz, Merle Arrowsmith, Maximilian Dietz, Stephan Hagspiel and Holger Braunschweig*

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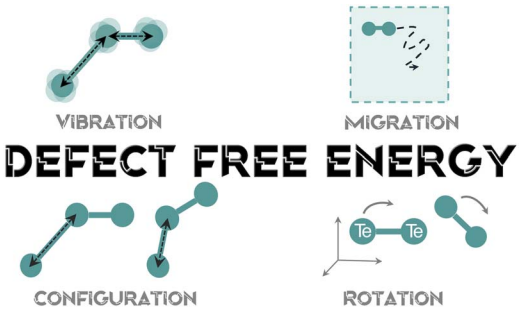
Point defect formation at finite temperatures with machine learning force fields

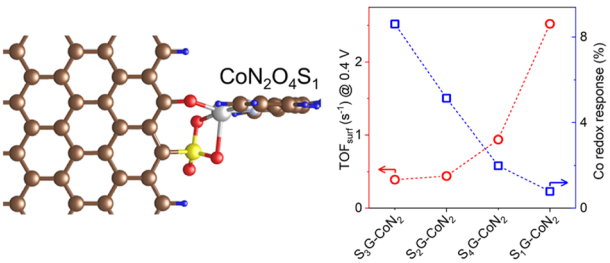
Irea Mosquera-Lois, Johan Klarbring and Aron Walsh*



8889

Tuning the electrochemical redox-mediated mechanism of oxygen evolution on cobalt sites by hydroxide ion coupling

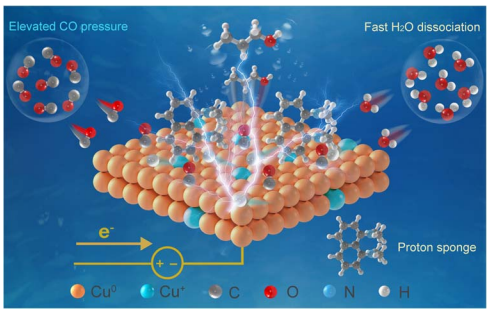
Wenjuan Song, Xiaoyue Duan, Poe Ei Phyu Win, Xiang Huang* and Jiong Wang*



8897

Cooperative promotion of electroreduction of CO to *n*-propanol by *CO enrichment and proton regulation

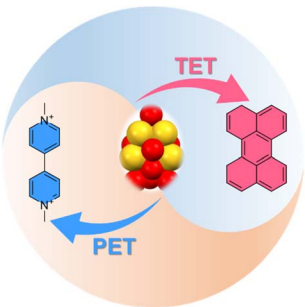
Rongxing Qiu, Linxiao Cui, Li Peng,* Olga A. Syzgantseva, Jiaran Li, Nan Fang, Maria A. Syzgantseva, Yuan Jiang, Jie Zhang, Bingxing Zhang, Lingzhi Ding, Yangyang Dong, Tianwei Xue, Cheng Li, Jin-Chao Dong, Jinyu Ye, Isil Akpinar, Shuliang Yang,* Jun Li,* Jianling Zhang, Jian-Feng Li and Buxing Han*



8910

Intensive near-infrared emitting Au_7Cu_{10} nanoclusters for both energy and electron harvesting

Wei Zhang, Tingting Xu, Jie Kong, Yuanming Li, Xiaoguo Zhou, Jiachen Zhang, Qun Zhang, Yongbo Song,* Yi Luo* and Meng Zhou*



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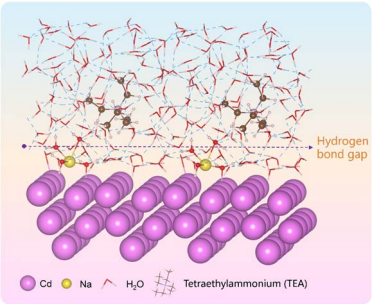
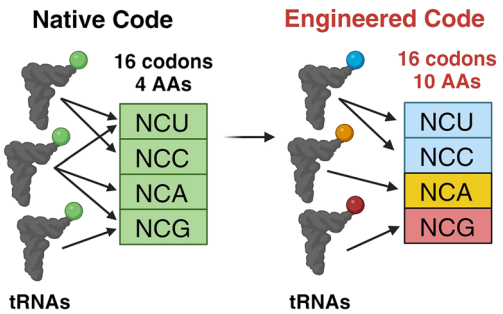


Promotion or suppression of hydrogen evolution activity? The competition between sodium cations and quaternary ammonium ions at the metal/water interface

Shilin Bo, Yang Xiang, Qiong Xiang, Li Li, Xun Huang* and Zidong Wei*

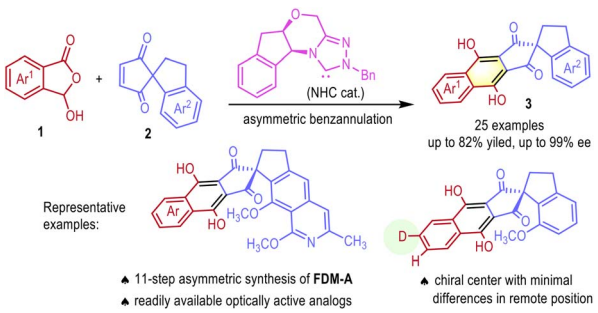
8932



Removing redundancy of the NCN codons *in vitro* for maximal sense codon reassignment

Clark A. Jones, Chelsea A. Makovsky, Aidan K. Haney, Alba C. Dutra, Clinton A. L. McFeely, T. Ashton Cropp and Matthew C. T. Hartman*

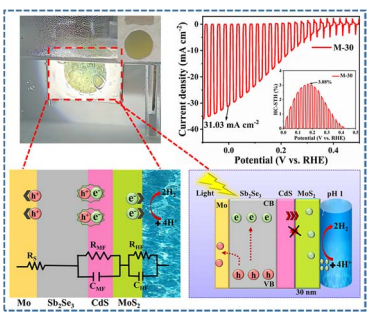
8940



Carbene-catalyzed enantioselective construction of a quasi-symmetrical spirocyclic hydroquinone with a minor chiral distinction

Panlong Ren, Qing Zhao, Yonggui Robin Chi* and Tingshun Zhu*

8946



Pt-free MoS_2 co-catalyst enables record photocurrent density in Sb_2Se_3 photocathodes for highly efficient solar hydrogen production

Munir Ahmad, Anadil Gul, Hafiz Sartaj Aziz, Tahir Imran, Muhammad Ishaq, Muhammad Abbas, Zhenghua Su and Shuo Chen*

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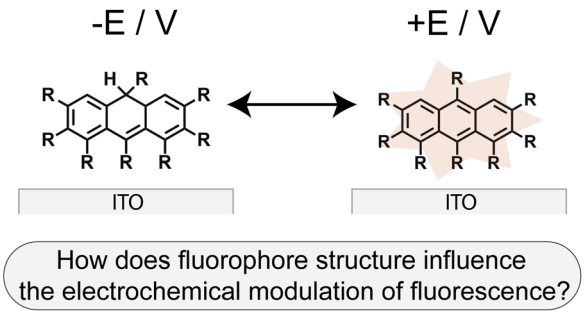
An investigative study of electrochemical induced fluorescence for fluorophores

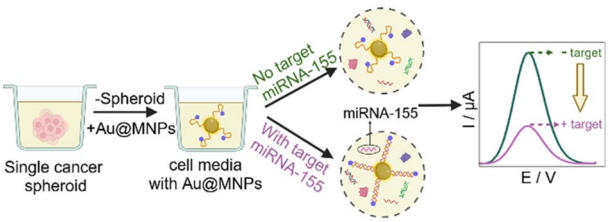
Daniel E. Hagness, Ying Yang, Yuanqing Ma, Sumaya Ishtiaq, Sanjun Fan, Richard D. Tilley* and J. Justin Gooding*



8970

Direct detection of microRNA in liquid biopsies from single cancer spheroids

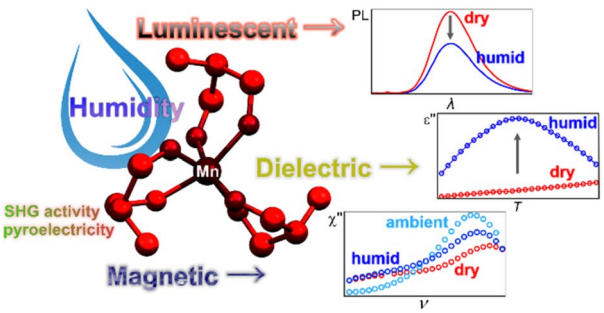
Chen Hu, Essam M. Dief, Bram G. Soliman, Sara Romanazzo, Shilpa Rana, Kristopher A. Kilian, Richard D. Tilley* and J. Justin Gooding*



8979

Photoluminescent, dielectric, and magnetic responsivity to the humidity variation in SHG-active pyroelectric manganese(II)-based molecular material

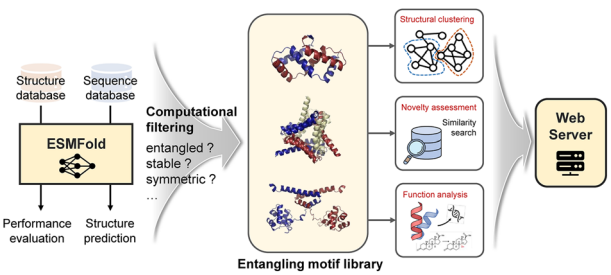
Aleksander Hoffman, Mikolaj Zychowicz, Junhao Wang, Keisuke Matsuura, Fumitaka Kagawa, Jan Rzepiela, Michal Heczko, Sebastian Baś, Hiroko Tokoro, Shin-ichi Ohkoshi and Szymon Chorazy*



8998

Computational discovery and systematic analysis of protein entangling motifs in nature: from algorithm to database

Puqing Deng, Yuxuan Zhang, Lianjie Xu, Jinyu Lyu, Linyan Li, Fei Sun, Wen-Bin Zhang* and Hanyu Gao*



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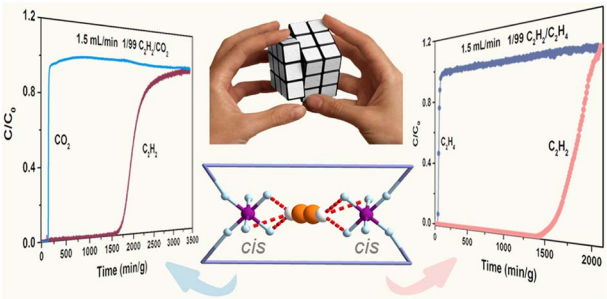
EDGE ARTICLES

9010



A new type of C_2H_2 binding site in a *cis*-bridging hexafluorosilicate ultramicroporous material that offers trace C_2H_2 capture

Bai-Qiao Song,* Mei-Yan Gao, Lisa Mercene van Wyk, Cheng-Hua Deng, Alan C. Eaby, Shi-Qiang Wang, Shaza Darwish, Dan Li, Shao-Jie Qin, Yun-Lei Peng,* Qing-Yuan Yang, Leonard J. Barbour and Michael J. Zaworotko*

9020

Facile post-synthesis of isomeric covalent organic frameworks *via* precise pore surface engineering

Yuhao Liu,* Yaze Chen, Ke Shi, Haijiao Peng and Chao Lu*

CORRECTION

9029

Correction: A comprehensive approach for elucidating the interplay between $4f^{n+1}$ and $4f^n5d^1$ configurations in Ln^{2+} complexes

Maria J. Beltran-Leiva, William N. G. Moore, Tener F. Jenkins, William J. Evans,* Thomas E. Albrecht* and Cristian Celis-Barros*

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