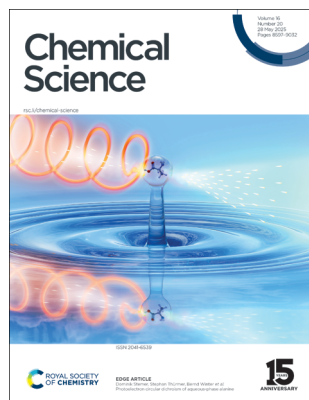


## IN THIS ISSUE

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.



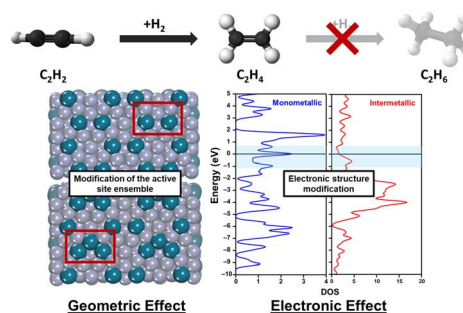
**Inside cover**  
See Haibo Xie *et al.*, pp. 8648–8660. Image reproduced by permission of Haibo Xie from *Chem. Sci.*, 2025, **16**, 8648.

## 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\*

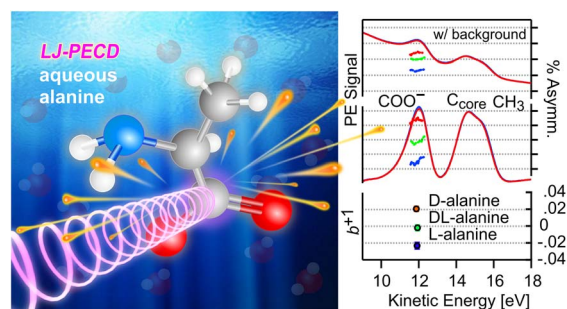


## EDGE ARTICLES

8637

### Photoelectron circular dichroism of aqueous-phase alanine

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



# EES Catalysis

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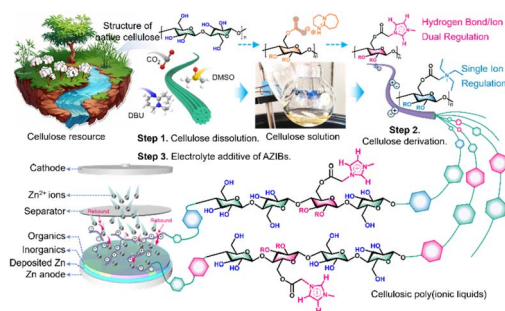
[rsc.li/EESCatalysis](https://rsc.li/EESCatalysis)

Fundamental questions  
Elemental answers

8648

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

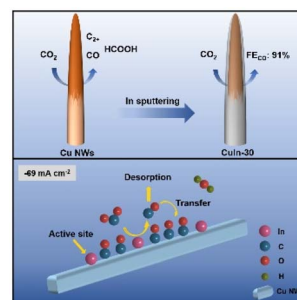
Kui Chen, Yongzhen Xu, Hebang Li, Yue Li, Lihua Zhang, Yuanlong Guo, Qinqin Xu, Yunqi Li and Haibo Xie\*



8661

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

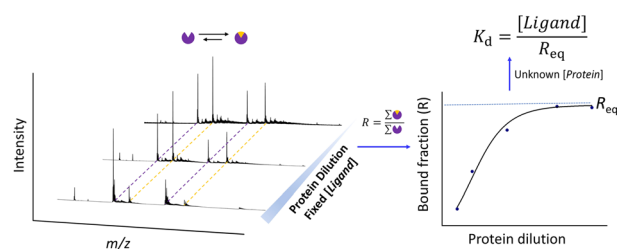
Shengzhou Xu, Chenglong Wang, Chunjing Ran, Hexing Yang, Wangjiang Gao, Bitao Dong,\* Yuhang Liu and Dan Ren\*



8673

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

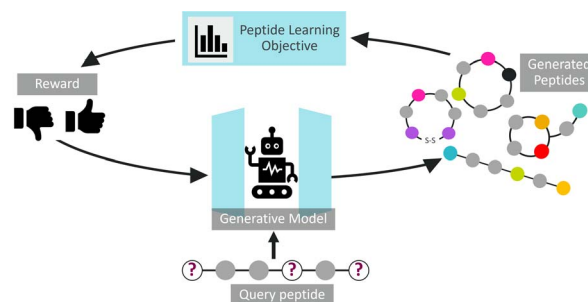
Bin Yan\* and Josephine Bunch\*



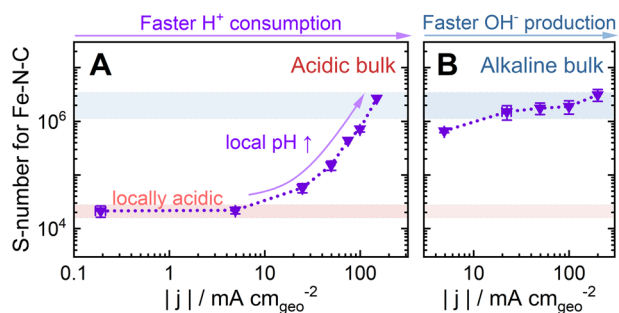
8682

## 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



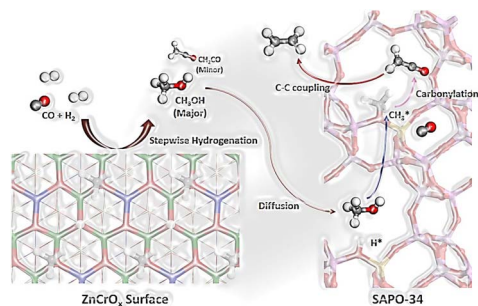
8697



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

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

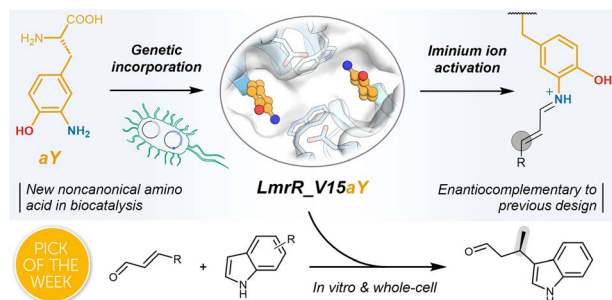
8711



### Unraveling the mechanisms of ketene generation and transformation in syngas-to-olefin conversion over ZnCrO<sub>x</sub>|SAPO-34 catalysts

Zhuo-Yan Yao, Sicong Ma<sup>\*</sup> and Zhi-Pan Liu<sup>\*</sup>

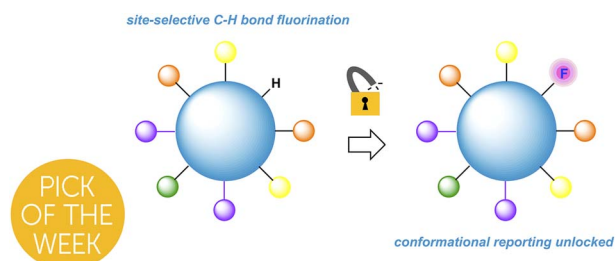
8721



### 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<sup>\*</sup>

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,<sup>\*</sup> Adam Huczyński and Thomas Lectka<sup>\*</sup>

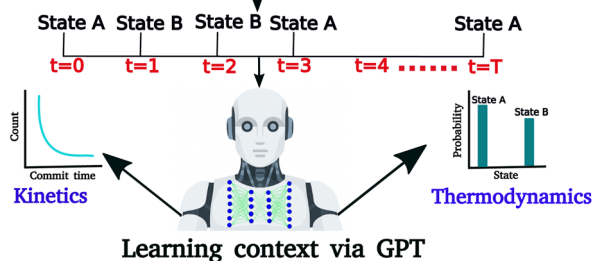


8735

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

Palash Bera\* and Jagannath Mondal\*

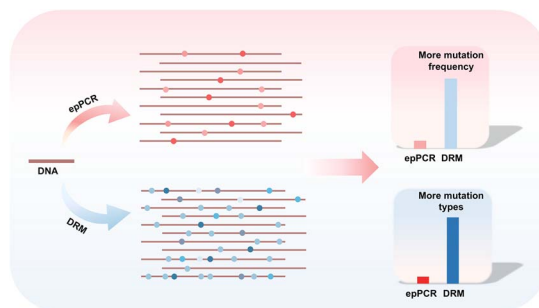
### Molecular Dynamics simulation trajectory



8752

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

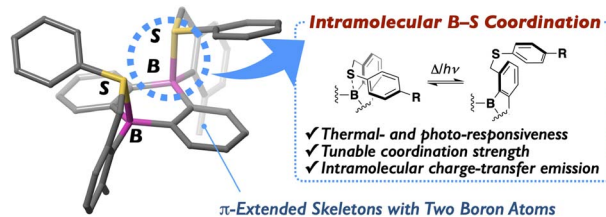
Ying Hao, Tong-Tong Ji, Shu-Yi Gu, Shan Zhang, Yao-Hua Gu, Xia Guo, Li Zeng, Fang-Yin Gang, Jun Xiong, Yu-Qi Feng,\* Neng-Bin Xie\* and Bi-Feng Yuan\*



8764

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

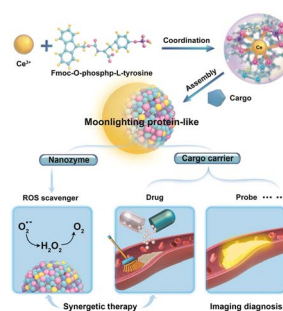
Hiroki Narita, Alexander Virovets, Hans-Wolfram Lerner, Matthias Wagner and Shigehiro Yamaguchi\*



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\*

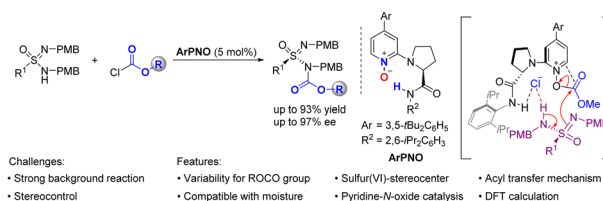




8812

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

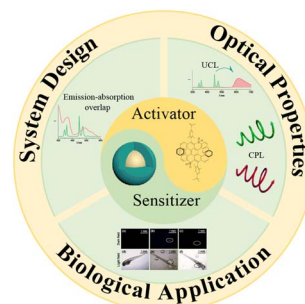
Cui-Mei Guo, Fang-Yuan Zhang, Yin Tian,\*  
Ming-Sheng Xie\* and Hai-Ming Guo\*



8820

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

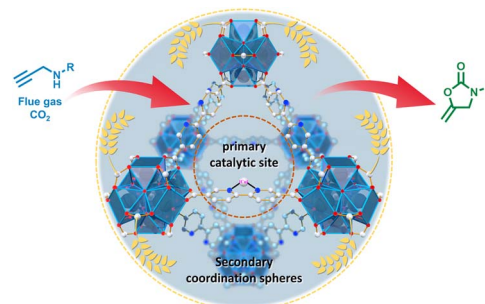
Jiangshan Luo, Junjian Shen, Xingwen Cheng,\* Yan Liu,  
Xiulian Yin, Tianxi Hu, Guangxin Fan, Jianming Zhang,  
Wei Zheng\* and Xueyuan Chen\*



8827

### Tailored engineering of primary catalytic sites and secondary coordination spheres in metalloenzyme-mimetic MOF catalysts for boosting efficient CO<sub>2</sub> conversion

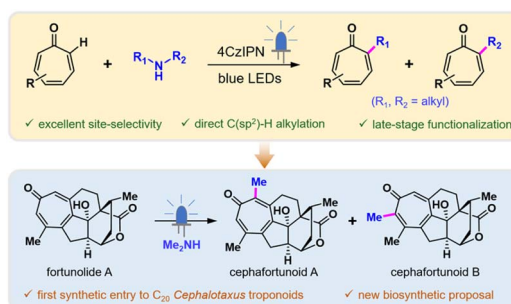
Jiawei Li,\* Fan Yang, Benling Yu, Zhongke Dai,  
Shiyuan Wei, Ying Wu,\* Liuqing He, Fa Zhou,  
Jianhan Huang\* and You-Nian Liu



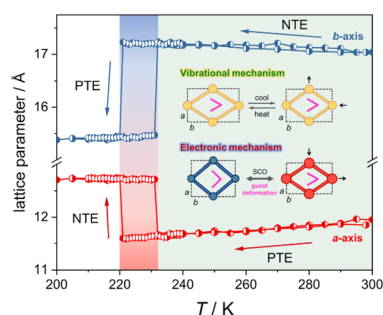
8836

### Visible-light-mediated site-selective C(sp<sup>2</sup>)-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\*



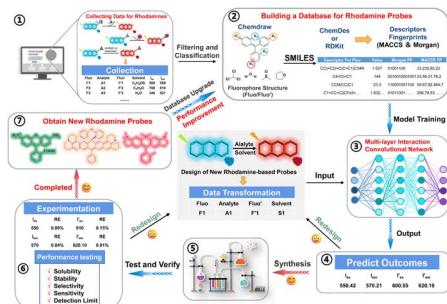
8845



### 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\*

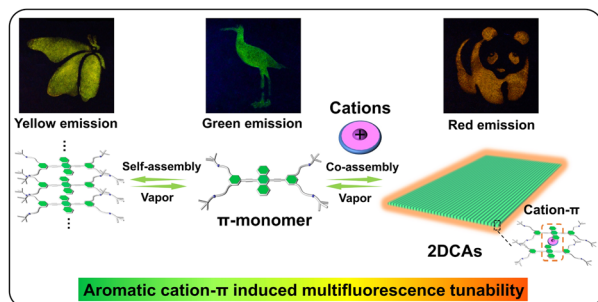
8853



### 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\*

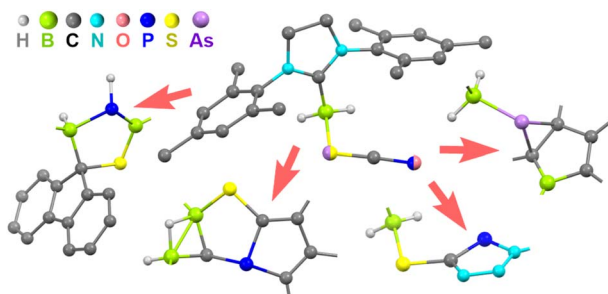
8861



### Aromatic cation- $\pi$ 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

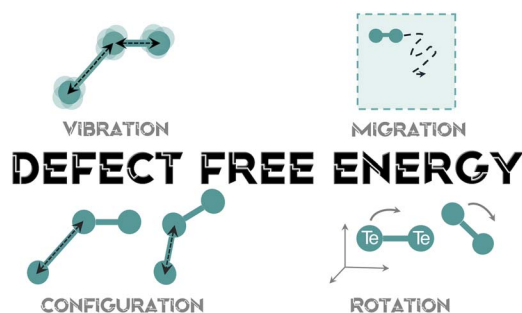
Malte Jürgensen, Tanja Kunz, Merle Arrowsmith, Maximilian Dietz, Stephan Hagspiel and Holger Braunschweig\*



8878

### Point defect formation at finite temperatures with machine learning force fields

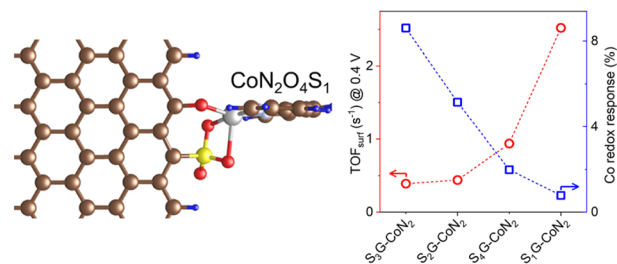
Irea Mosquera-Lois, Johan Klarbring and Aron Walsh\*



8889

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

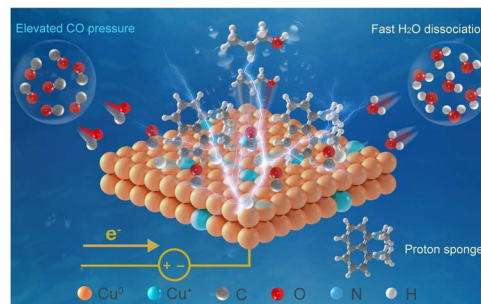
Wenjuan Song, Xiaoyue Duan, Poe Ei Phyu Win, Xiang Huang\* and Jiong Wang\*



8897

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

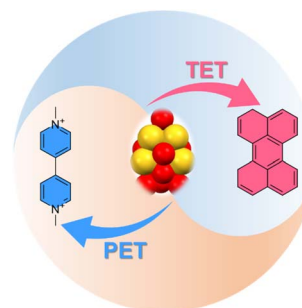
Rongxing Qiu, Linxiao Cui, Li Peng,\* Olga A. Syzgantseva, Jiaran Li, Nan Fang, Maria A. Syzgantseva, Yuan Jiang, Jie Zhang, Bingxing Zhang, Lingzhi Ding, Yangyang Dong, Tianwei Xue, Cheng Li, Jin-Chao Dong, Jinyu Ye, Isil Akpınar, Shuliang Yang,\* Jun Li,\* Jianling Zhang, Jian-Feng Li and Buxing Han\*



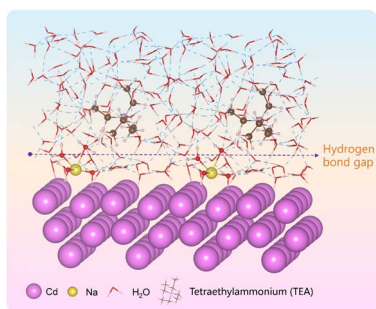
8910

### Intensive near-infrared emitting Au<sub>7</sub>Cu<sub>10</sub> 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\*



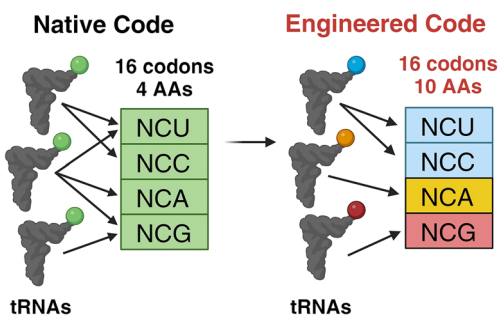
8922



### 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\*

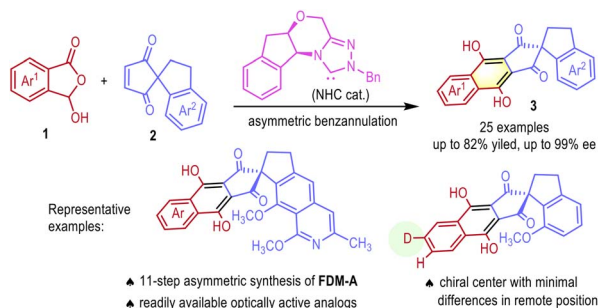
8932



### 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\*

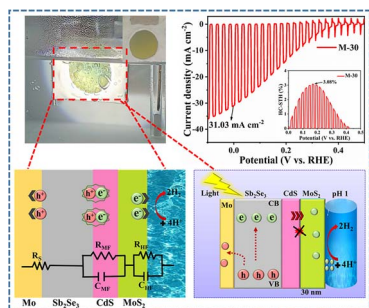
8940



### 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<sub>2</sub> co-catalyst enables record photocurrent density in Sb<sub>2</sub>Se<sub>3</sub> photocathodes for highly efficient solar hydrogen production

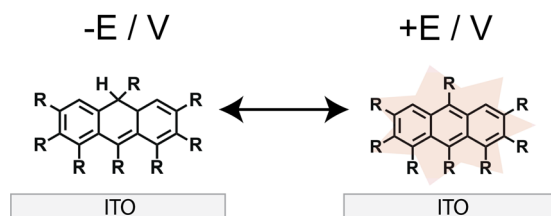
Munir Ahmad, Anadil Gul, Hafiz Sartaj Aziz, Tahir Imran, Muhammad Ishaq, Muhammad Abbas, Zhenghua Su and Shuo Chen\*



8959

### 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\*

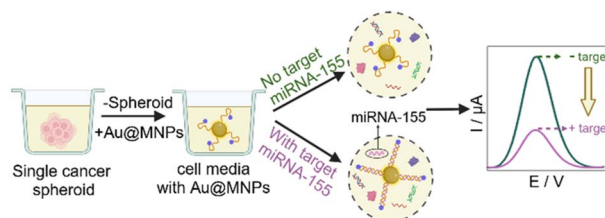


How does fluorophore structure influence the electrochemical modulation of fluorescence?

8970

### Direct detection of microRNA in liquid biopsies from single cancer spheroids

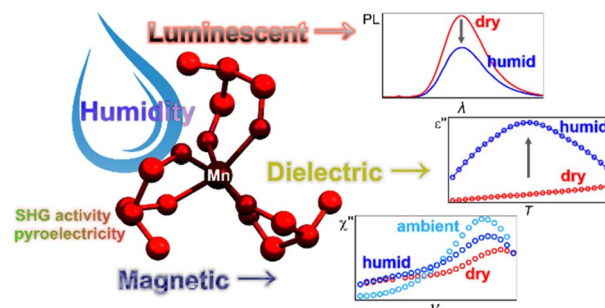
Chen Hu, Essam M. Dief, Bram G. Soliman, Sara Romanazzo, Shilpa Rana, Kristopher A. Kilian, Richard D. Tilley\* and J. Justin Gooding\*



8979

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

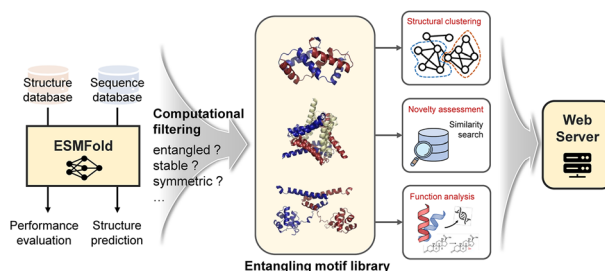
Aleksander Hoffman, Mikolaj Zychowicz, Junhao Wang, Keisuke Matsuura, Fumitaka Kagawa, Jan Rzepiela, Michal Heczko, Sebastian Baś, Hiroko Tokoro, Shin-ichi Ohkoshi and Szymon Chorazy\*



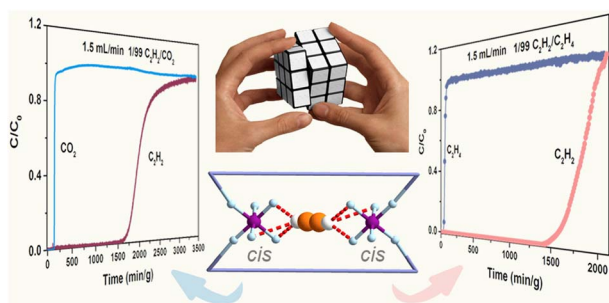
8998

### 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\*



9010



### A new type of C<sub>2</sub>H<sub>2</sub> binding site in a *cis*-bridging hexafluorosilicate ultramicroporous material that offers trace C<sub>2</sub>H<sub>2</sub> capture

Bai-Qiao Song,<sup>\*</sup> 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,<sup>\*</sup> Qing-Yuan Yang, Leonard J. Barbour and Michael J. Zaworotko<sup>\*</sup>

9020



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

Yuhao Liu,<sup>\*</sup> Yaze Chen, Ke Shi, Haijiao Peng and Chao Lu<sup>\*</sup>

9029

### Correction: A comprehensive approach for elucidating the interplay between 4f<sup>n+1</sup> and 4f<sup>n</sup>5d<sup>1</sup> configurations in Ln<sup>2+</sup> complexes

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

