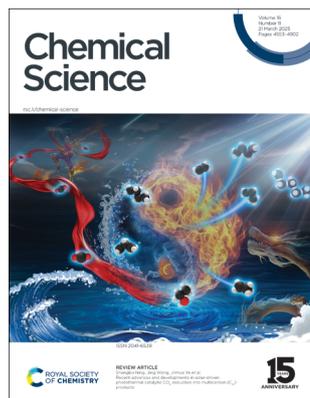


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ISSN 2041-6539 CODEN CSHCBM 16(11) 4553–4902 (2025)



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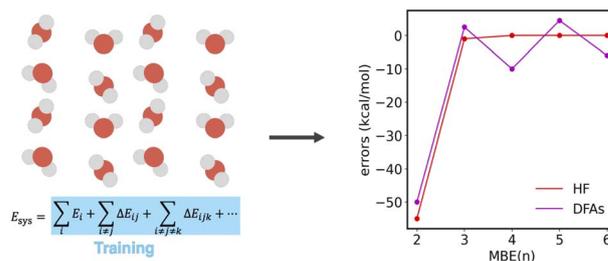
**Inside cover**  
See Simone Scintilla, Sheref S. Mansy *et al.*, pp. 4614–4624. Image reproduced by permission of Sheref S. Mansy from *Chem. Sci.*, 2025, **16**, 4614. Artwork created by Annie Tykwinski.

## COMMENTARY

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### A focus on delocalization error poisoning the density-functional many-body expansion

Barbaro Zulueta and John A. Keith\*

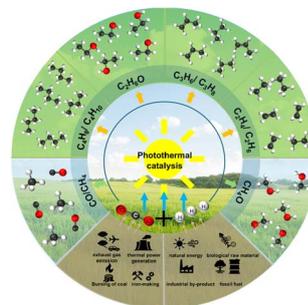


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### Recent advances and developments in solar-driven photothermal catalytic CO<sub>2</sub> reduction into multicarbon (C<sub>2+</sub>) products

Xiuting Wu, Senlin Zhang, Shangbo Ning,\* Chuanyun Yang, Ling Li, Linjun Tang, Jing Wang,\* Ruixiang Liu, Xingyu Yin, Ying Zhu, Shaohua Chen and Jinhua Ye\*



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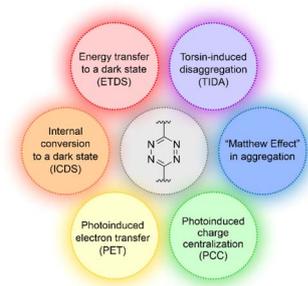
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## REVIEWS

4595

## Unveiling the photophysical mechanistic mysteries of tetrazine-functionalized fluorogenic labels

Tianruo Shen and Xiaogang Liu\*

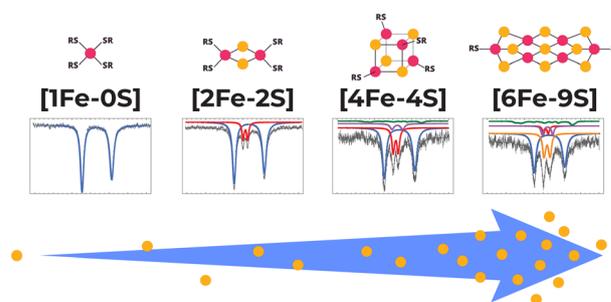


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## Prebiotic synthesis of the major classes of iron–sulfur clusters

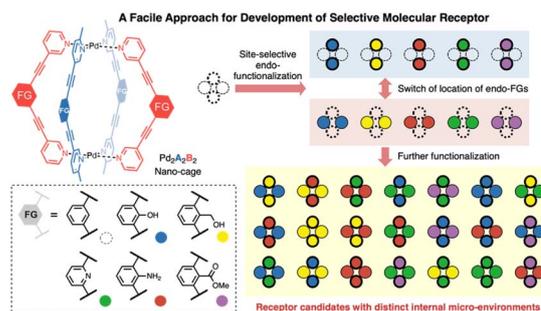
Simone Scintilla,\* Daniele Rossetto, Martin Clémancey, Julia Rendon, Antonio Ranieri, Graziano Guella, Michael Assfalg, Marco Borsari, Serge Gambarelli, Geneviève Blondin and Sheref S. Mansy\*



4625

## Precise functionalization in nano-confinement: a bottom-up approach to the evolution of selective molecular receptors

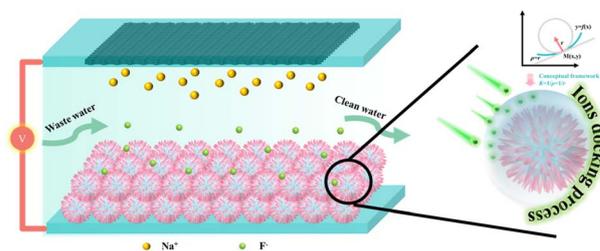
Ya-Mei Tan, Lu-Mei Zhang, Qixia Bai, Zhe Zhang, Pingshan Wang and Qi Zhang\*



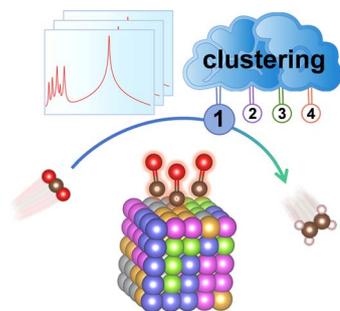
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Curvature enhanced NH<sub>2</sub>-MIL-53(Al) electrode for boosting ion diffusion and capacitive deionization defluorination

Fei Yu, Yidi Yang, Peng Liu and Jie Ma\*



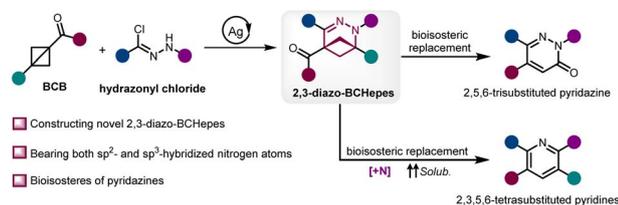
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### Spectra-based clustering of high-entropy alloy catalysts: improved insight over use of atomic structure

Huirong Li, Donglai Zhou, Pieter E. S. Smith, Edward Sharman, Hengyu Xiao, Song Wang,\* Yan Huang\* and Jun Jiang\*

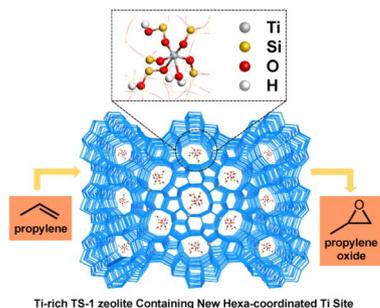
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### Silver-mediated formal $[4\pi + 2\sigma]$ cycloaddition reactions of bicyclobutanes with nitrile imines: access to 2,3-diazobicyclo[3.1.1]heptenes

Huijuan Liao, Jianyang Dong,\* Xuechen Zhou, Qin Jiang, Zishan Lv, Fang Lei and Dong Xue\*

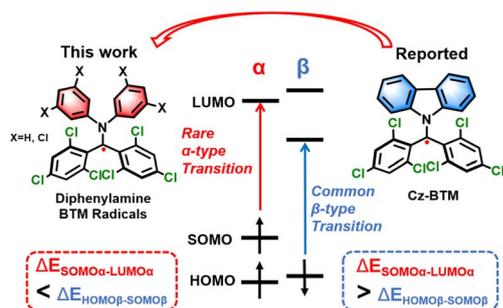
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### Ethanol-assisted synthesis of titanium-rich TS-1 zeolite: a new hexa-coordinated Ti site for efficient propylene epoxidation

Dapeng Hao, Xintong Li, Guangyuan He, Risheng Bai, Yang Bai, Tianjun Zhang, Lisu Bai, Jialiang Li, Qiang Zhang, Donghai Mei, Zhaochi Feng\* and Jihong Yu\*

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### Stable luminescent diphenylamine biphenylmethyl radicals with $\alpha$ -type $D_0 \rightarrow D_1$ transition and antiferromagnetic properties

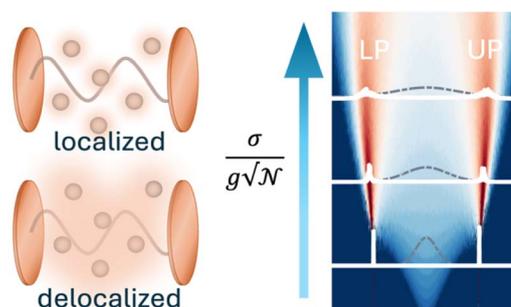
Shengxiang Gao, Chunxiao Wu, Ming Zhang and Feng Li\*



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### Unlocking delocalization: how much coupling strength is required to overcome energy disorder in molecular polaritons?

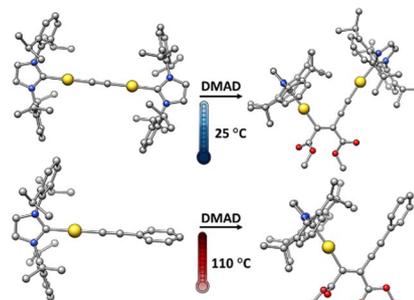
Tianlin Liu, Guoxin Yin and Wei Xiong\*



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### Stepwise alkyne insertion in Au(I) acetylides: influence of the nuclearity

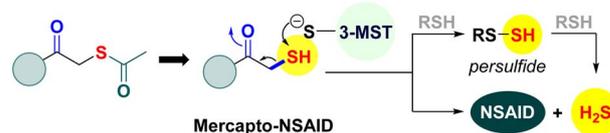
Juan Cayuela-Castillo, Francisco J. Fernández-de-Córdova, Matthew S. See, Israel Fernández\* and Pablo Ríos\*



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### Mercapto-NSAIDs generate a non-steroidal anti-inflammatory drug (NSAID) and hydrogen sulfide

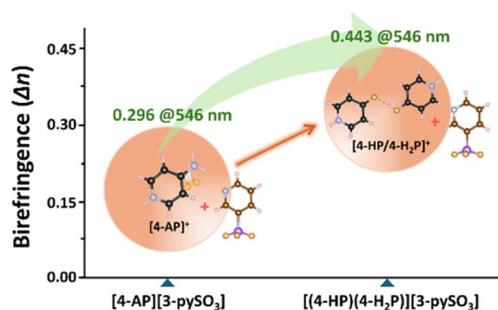
Simran M. Gupta, Pratiksha S. Mohite and Harinath Chakrapani\*



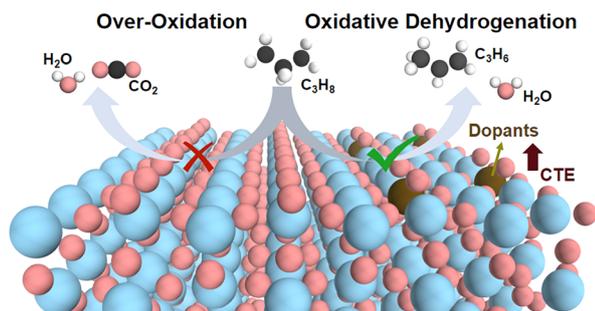
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### Synergistic engineering of ultraviolet metal-free crystals with exceptional birefringence via pyridine-derived dimers

Jiachen Lu and Kang Min Ok\*



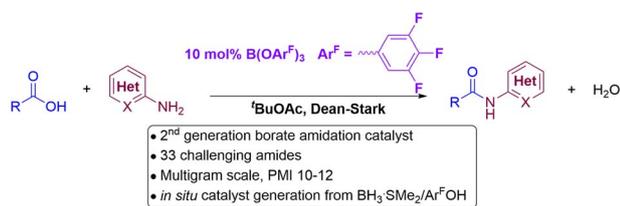
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### Role and regulation of surface oxygen vacancies in vanadium-based oxides for chemical looping oxidative dehydrogenation of propane

Dehui Luo, Ran Luo, Xianhui Wang, Xin Chang, Tingting Yang, Sai Chen, Zhi-Jian Zhao\* and Jinlong Gong\*

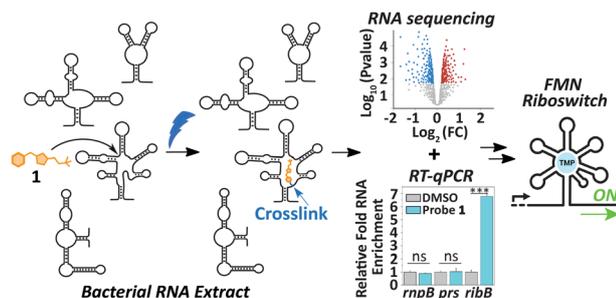
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### Borate-catalysed direct amidation reactions of coordinating substrates

Richard J. Procter, Carla Alamillo-Ferrer, Usman Shabbir, Phyllida Britton, Dejan-Krešimir Bučar, Alexandre S. Dumon, Henry S. Rzepa,\* Jordi Burés,\* Andrew Whiting\* and Tom D. Sheppard\*

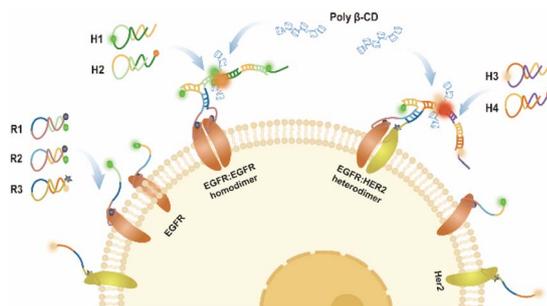
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### Chemotranscriptomic profiling with a thiamine monophosphate photoaffinity probe

Stefan Crielaard, Casper F. M. Peters, Alexandar Slivkov, Daphne A. L. van den Homberg and Willem A. Velema\*

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### A supramolecular FRET signal amplification nanoprobe for high contrast and synchronous *in situ* imaging of cell surface receptor homodimers/heterodimers

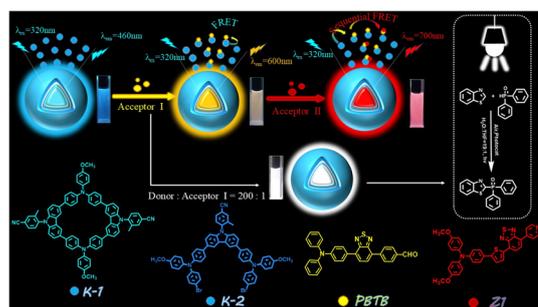
Ya Wang, Feng Yao, Lulu Song, Mengpan Zhang, Zitong Gong, Yunli Zhao, Yamin Xiong\* and Leiliang He\*



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### Novel supramolecular artificial light-harvesting systems based on AIE-active macrocycles for efficient white-light photocatalysis in water

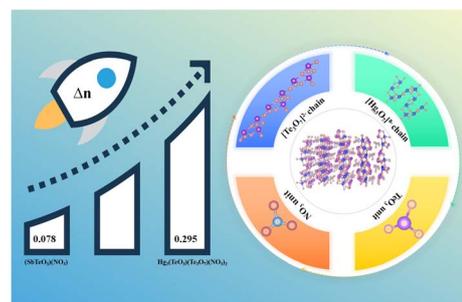
Jun-Cheng Yang, Ke Chen, Guo-Ling Zhang, Chunxuan Qi, Hai-Tao Feng\* and Ben Zhong Tang\*



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### "All-four-in-one": a novel mercury tellurite-nitrate $\text{Hg}_3(\text{TeO}_3)(\text{Te}_3\text{O}_7)(\text{NO}_3)_2$ exhibiting exceptional optical anisotropy

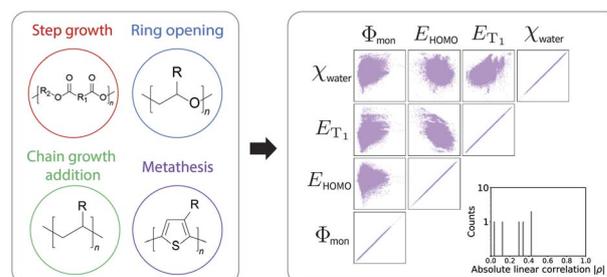
Ru-Ling Tang,\* Yi-Lei Lv, Liang Ma, Bing-Wei Miao, Wenlong Liu and Sheng-Ping Guo\*



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### Functional monomer design for synthetically accessible polymers

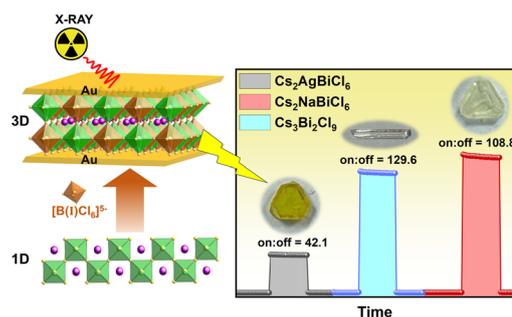
Seonghwan Kim, Charles M. Schroeder and Nicholas E. Jackson\*



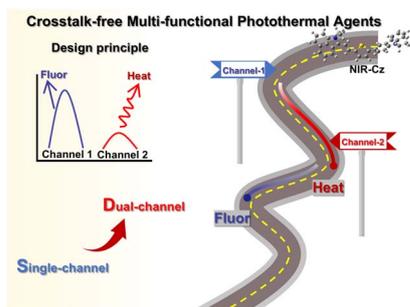
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### Highly stable bismuth-chloride perovskite X-ray direct detectors with an ultralow detection limit

Haoyu Chen, Qingyun Han, Haoming Qin, Yueqi Shen, Huijun Lv, Yan Liu, Liping Du, Yong Wang, Yihui He\* and Weihua Ning\*



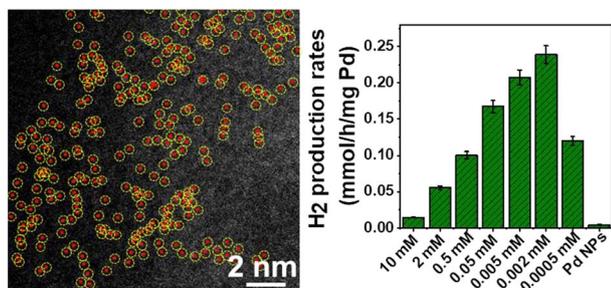
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### Construction of crosstalk-free multi-functional phototherapeutic agents

Lixuan Dai, Wenxiu Li, Xiaoli Zhong, Mingguang Ren, Tony D. James\* and Weiyang Lin\*

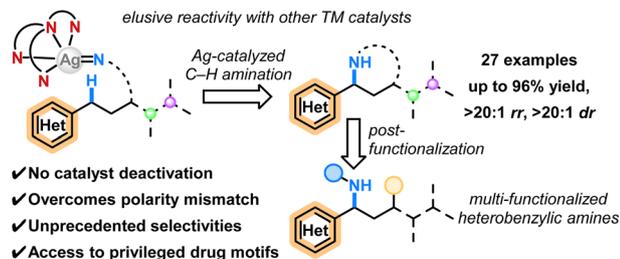
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### Pd single atoms on g-C<sub>3</sub>N<sub>4</sub> photocatalysts: minimum loading for maximum activity

Velu Jeyalakshmi, Siming Wu, Shanshan Qin, Xin Zhou, Bidyut Bikash Sarma, Dimitry E. Doronkin, Jan Kolařík, Miroslav Šooš and Patrik Schmuki\*

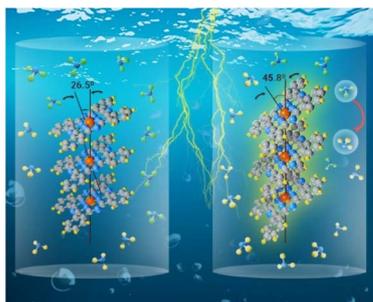
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### Site- and stereoselective silver-catalyzed intramolecular amination of electron-deficient heterobenzylic C-H bonds

Tuan Anh Trinh, Stanislav Cherempei, Daniel S. Rampon and Jennifer M. Schomaker\*

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### Controlling electrocatalytic nitrate reduction efficiency by utilizing d $\pi$ -p $\pi$ interactions in parallel stacking molecular systems

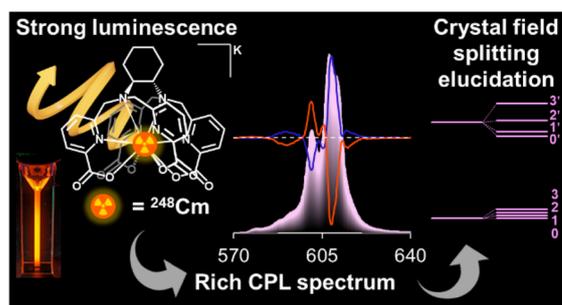
Sourav Bhowmick, Ashadul Adalder, Abhishek Maiti, Samadhan Kapse, Ranjit Thapa, Supriya Mondal and Uttam Kumar Ghora\*



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### Room temperature crystal field splitting of curium resolved by circularly polarized luminescence spectroscopy

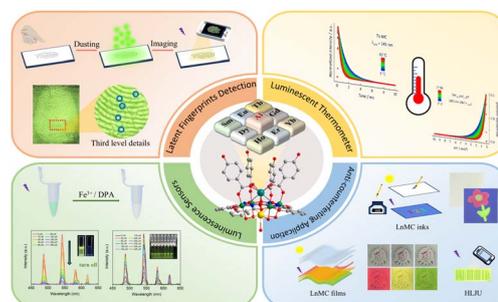
Joshua J. Woods, Appie Peterson, Joseph A. Adewuyi, Rachael Lai, Jennifer N. Wacker, Rebecca J. Abergel\* and Gaël Ung\*



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### A novel Ln<sup>3+</sup>/Al<sup>3+</sup> metallacrown multifunctional material for latent fingerprint detection, luminescent thermometers and luminescent sensors

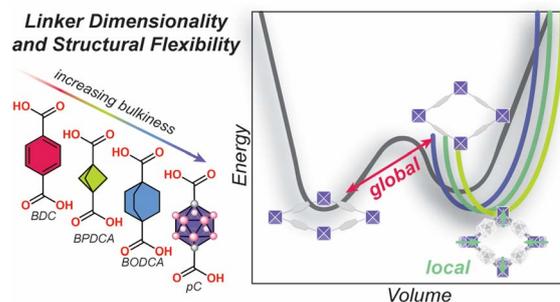
Han Yan, Claudia M. S. Calado, Hao Wang, Muralee Murugesu\* and Wen-Bin Sun\*



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### Exceeding flexexpectations: a combined experimental and computational investigation of structural flexibility in 3-dimensional linker-based metal-organic frameworks

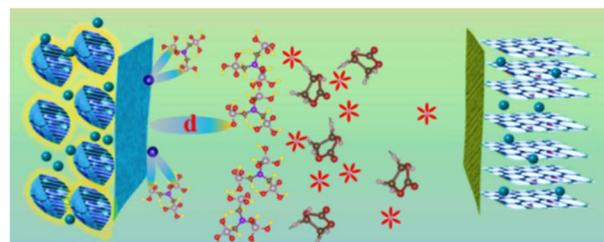
Courtney S. Smoljan, Filip Formalik, Michael L. Barsoum, Kira M. Fahy, Madeleine A. Gaidimas, Florencia A. Son, Haomiao Xie, Karam B. Idrees, Omar K. Farha\* and Randall Q. Snurr\*



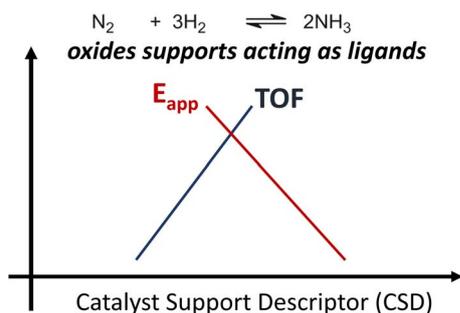
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### Inhibiting homogeneous catalysis of cobalt ions towards stable battery cycling of LiCoO<sub>2</sub> at 4.6 V

Chao Sun, Bing Zhao, Qing Wen, Xiang-tao Chen, Ning-yun Hong, Jin-bo Zeng, Jia-feng Zhang, Ling-jun Li, Jie-xi Wang, Xia-hui Zhang and Jun-chao Zheng\*



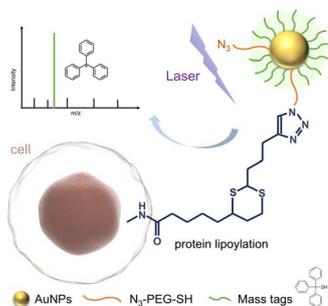
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### A descriptor guiding the selection of catalyst supports for ammonia synthesis

Andreas Weilhard, Ilya Popov, Emerson C. Kohlrausch, Gazi N. Aliev, L. Scott Blankenship, Luke T. Norman, Sadegh Ghaderzadeh, Louise Smith, Mark Isaacs, James O'Shea, Anabel E. Lanterna, Wolfgang Theis, David Morgan, Graham J. Hutchings, Elena Besley, Andrei N. Khlobystov and Jesum Alves Fernandes\*

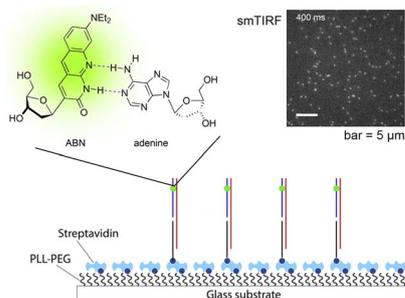
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### Chemoselective and laser cleavable probes for *in situ* protein lipoylation detection by laser desorption/ionization mass spectrometry

Qiuyao Du, Xi Yu, Ke Jia, Yijiao Qu, Jing Han, Jiameng Sun, Duo Shen, Huihui Liu and Zongxiu Nie\*

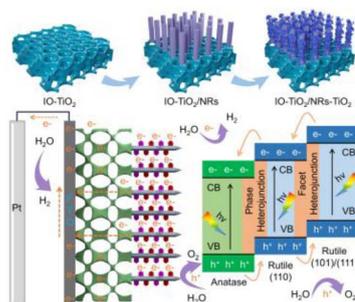
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### Single-molecule detection of oligonucleotides using the fluorescent nucleobase analogue ABN

George N. Samaan, Andres Jimenez Salinas, Alexandra E. Bailie, Julian Grim, Julian M. Cizmic, Anita C. Jones,\* Youngkwang Lee\* and Byron W. Purse\*

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### Inverse opal anatase/rutile TiO<sub>2</sub> multi-heterojunctions enable efficient photoelectrochemical water splitting

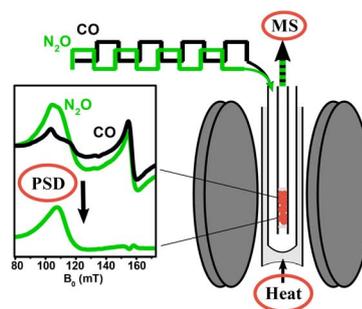
Bo-Hao Xiao, Chen Huo, Jin-Yu Chen, Ying-Guan Xiao, Shun-Sheng Cao\* and Zhao-Qing Liu\*



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### Elucidation of site-specific red-ox kinetics in the CO-assisted $N_2O$ decomposition over Fe-ferrierite by combining modulation excitation with *operando* EPR spectroscopy

Jörg W. A. Fischer, Filippo Buttignol, Alberto Garbujo, Davide Ferri\* and Gunnar Jeschke\*



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### Protein-cell conjugates as artificial surface display for interfacial biocatalysis

Xiankun Wu, Henrik Karring, Zhongkai Wang\* and Changzhu Wu\*

