

# Chemical Science

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## IN THIS ISSUE

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**Cover**  
See Koki Ikemoto, Hiroyuki Isobe *et al.*, pp. 3045–3050. Image reproduced by permission of Koki Ikemoto, Misato Akiyoshi and Hiroyuki Isobe from *Chem. Sci.*, 2025, **16**, 3045.



**Inside cover**  
See Heidi M. Quitián-Lara, Felipe Fantuzzi, Albeiro Restrepo *et al.*, pp. 3051–3065. Image reproduced by permission of Felipe Fantuzzi from *Chem. Sci.*, 2025, **16**, 3051.

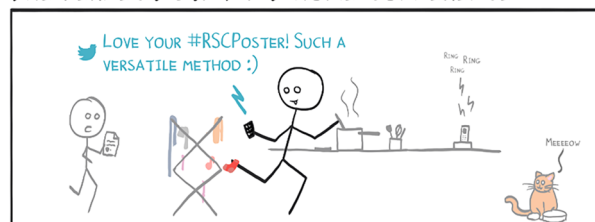
## EDITORIAL

2950

### Celebrating 10 years of #RSCPoster

Natalie Cotterell, Patrick A. J. M. de Jongh, Timothy Noël, Tanja Junkers, C. Malla Reddy, Athina Anastasaki and Edward Randviir

### THE PERFECT STAY-AT-HOME CONFERENCE



ROYAL SOCIETY OF CHEMISTRY

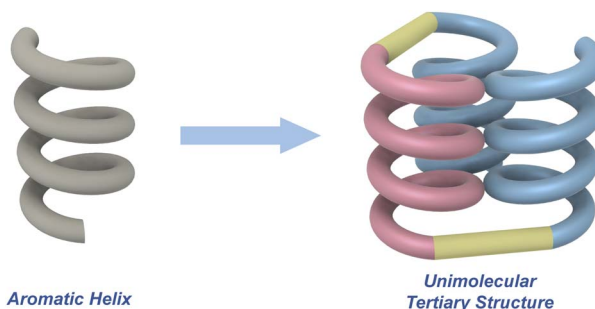
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## COMMENTARY

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### A focus on a complex abiotic tertiary structure

Yulong Zhong and Bing Gong\*



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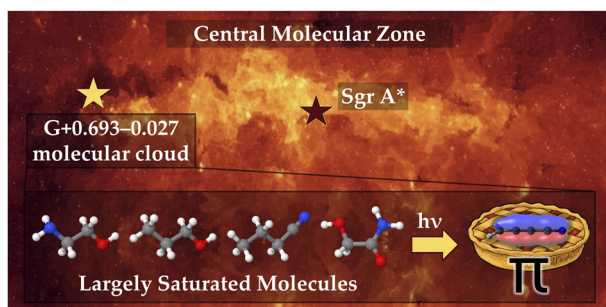
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Fundamental questions  
Elemental answers



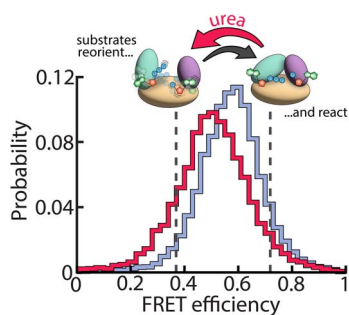
3051



### More $\pi$ , please: What drives the formation of unsaturated molecules in the interstellar medium?

Jhoan Londoño-Restrepo, Santiago Gómez, Heidi M. Quitián-Lara,\* Felipe Fantuzzi\* and Albeiro Restrepo\*

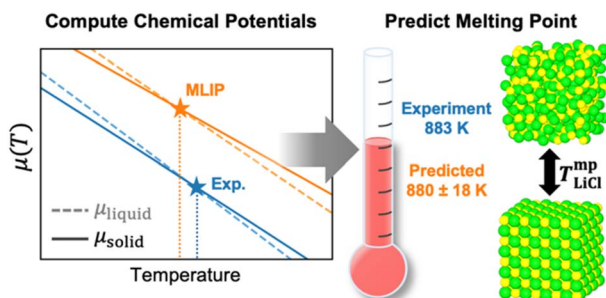
3066



### Interplay between conformational dynamics and substrate binding regulates enzymatic activity: a single-molecule FRET study

David Scheerer,\* Dorit Levy, Remi Casier, Inbal Riven, Hisham Mazal and Gilad Haran\*

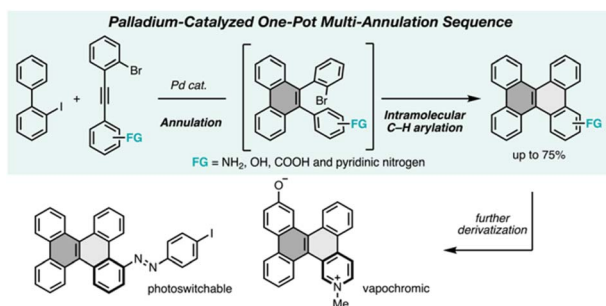
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### Computing chemical potentials with machine-learning-accelerated simulations to accurately predict thermodynamic properties of molten salts

Luke D. Gibson,\* Rajni Chahal and Vyacheslav S. Bryantsev\*

3092



### Rapid access to functionalized nanographenes through a palladium-catalyzed multi-annulation sequence

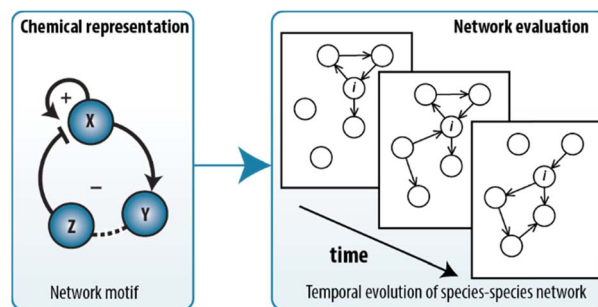
Takehisa Maekawa\* and Kenichiro Itami\*



3099

### Identify structures underlying out-of-equilibrium reaction networks with random graph analysis

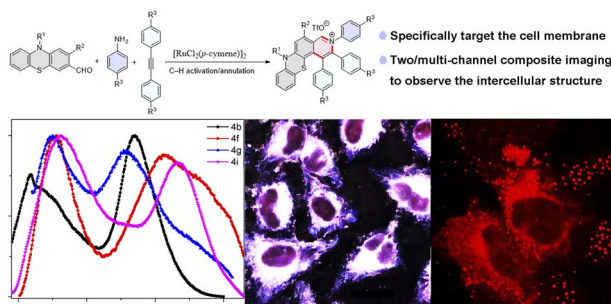
Éverton F. da Cunha, Yanna J. Kraakman, Dmitrii V. Kriukov, Thomas van Poppel, Clara Stegehuis\* and Albert S. Y. Wong\*



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### Ruthenium-catalyzed C–H bond activation and annulation of phenothiazine-3-carbaldehydes: facile access to dual-emission materials

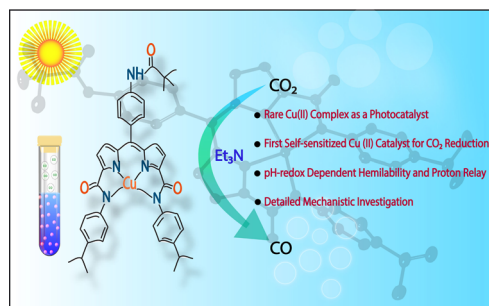
Junxiang Liu, Kangmin Wang, Liqiu Wan, Xianhui Yang and Bijin Li\*



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### Self-sensitized Cu(II)-complex catalyzed solar driven CO<sub>2</sub> reduction

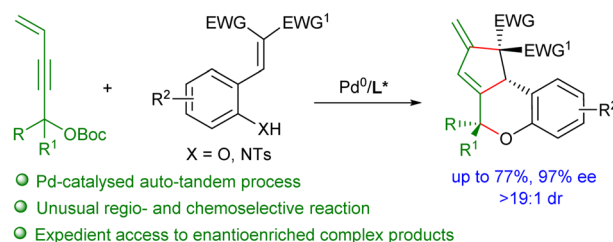
Soumadip Das, Aritra Roy, Navonil Chakrabarti, Narottam Mukhopadhyay, Aniruddha Sarkar and Sayam Sen Gupta\*



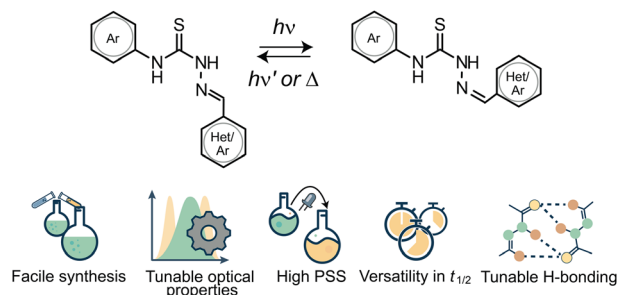
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### Palladium-catalysed asymmetric cascade transformations of 4-alken-2-ynyl carbonates to construct complex frameworks

Ze-Liang He, Li Li, Zhi-Chao Chen,\* Wei Du and Ying-Chun Chen\*



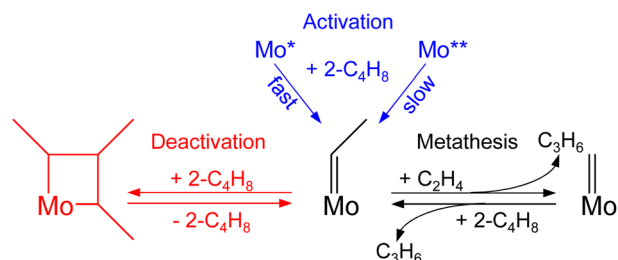
3130



### Thiosemicarbazones as versatile photoswitches with light-controllable supramolecular activity

Bengi Sentürk, Burkhard Butschke and Fabian Eisenreich\*

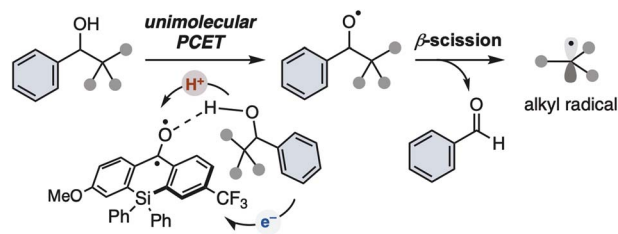
3141



### Time-resolved and theoretical analysis of Mo-carbene transformations in metathesis of ethylene with 2-butene

Tatiana Otroshchenko,\* Aleksandr Fedorov, Qiyang Zhang, David Linke, Jarostaw Handzlik, Mirjam Schröder, Björn Corzilius and Evgenii V. Kondratenko\*

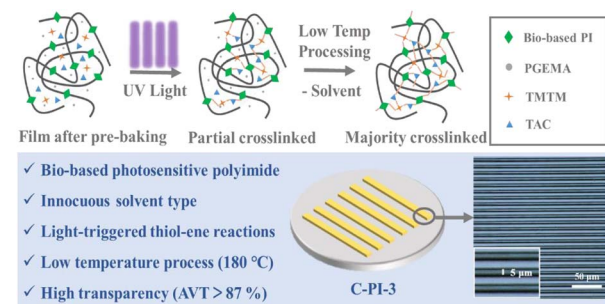
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### Organic photoredox-catalyzed unimolecular PCET of benzylic alcohols

Tomotoki Matsuo, Masaki Sano, Yuto Sumida\* and Hirohisa Ohmiya\*

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### Innocuous solvent-based, low-temperature curable, and highly transparent photosensitive polyimides developed using soluble polyimides containing bio-based magnolol moieties

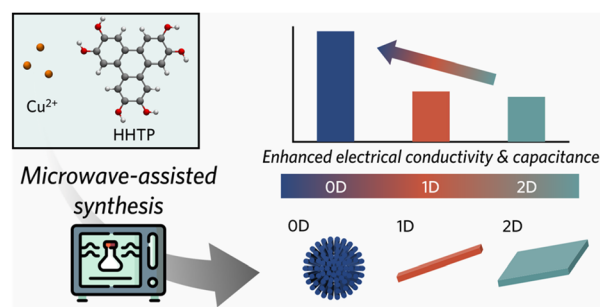
Huifa Meng, Kaijin Chen, Chuying Li, Longfei Zhang, Yanwei He, Zining Zhao, Peixin Wu, Hai Zhu, Zhenguo Chi, Jiarui Xu, Siwei Liu and Yi Zhang\*



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### From 0D to 2D: microwave-assisted synthesis of electrically conductive metal–organic frameworks with controlled morphologies

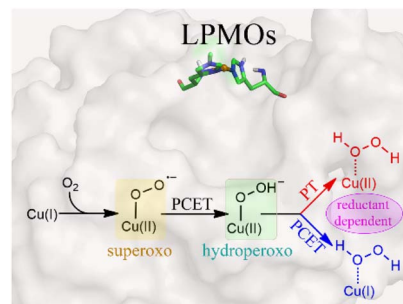
Xiaoyu Fang, Ji Yong Choi, Chenwei Lu, Elizabeth Reichert, Hoai T. B. Pham and Jihye Park\*



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### Theoretical study of the *in situ* formation of H<sub>2</sub>O<sub>2</sub> by lytic polysaccharide monoxygenases: the reaction mechanism depends on the type of reductant

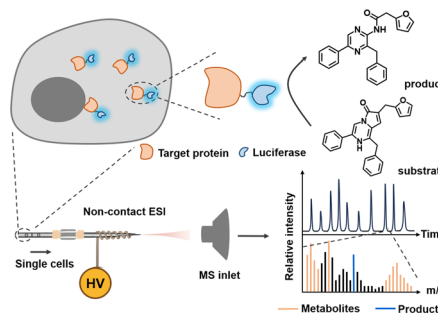
Zhanfeng Wang,\* Xiaodi Fu, Wenwen Diao, Yao Wu,\* Carme Rovira\* and Binju Wang\*



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### Multi-dimensional bio mass cytometry: simultaneous analysis of cytoplasmic proteins and metabolites on single cells

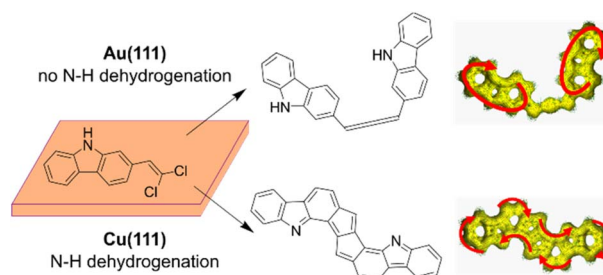
Shaojie Qin, Xinyi Zhang, Yi Zhang, Daiyu Miao, Wensheng Wei and Yu Bai\*



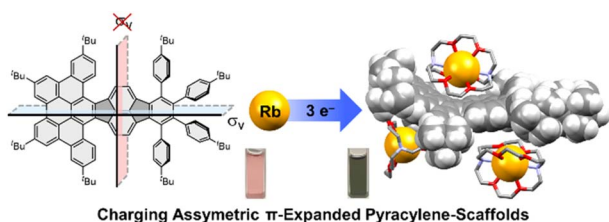
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### Competing pathways to aromaticity governed by amine dehydrogenation and metal–organic complexation in on-surface synthesis

Andrés Lombana, Songpol Chaunchaiyakul, Olivier Chuzel,\* Denis Hagebaum-Reignier, Jean-Luc Parrain,\* Franck Bocquet, Laurent Nony, Christian Loppacher, Federica Bondino, Elena Magnano, Hiroshi Imada, Emiko Kazuma, Yousoo Kim, Luca Giovanelli\* and Sylvain Clair\*



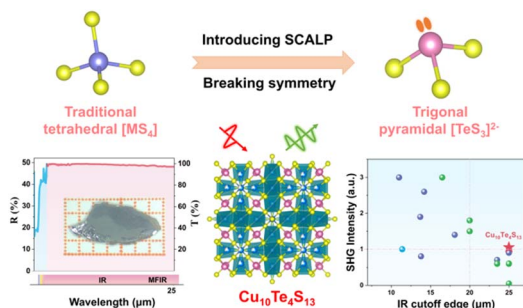
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### Stepwise reduction of an asymmetric $\pi$ -expanded pyracylene towards the crystalline radical trianion

Yikun Zhu, Jan Borstelmann, Christian Neiss, Zheng Wei, Andreas Göring, Milan Kivala\* and Marina A. Petrukhina\*

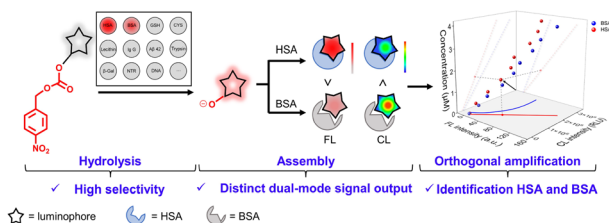
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### Exploring new horizons in mid-to-far infrared nonlinear optical crystals: the significant potential of trigonal pyramidal $[TeS_3]^{2-}$ functional units

Bo Zhang, Sheng-Hua Zhou,\* Bing-Xuan Li, Xin-Tao Wu, Hua Lin\* and Qi-Long Zhu\*

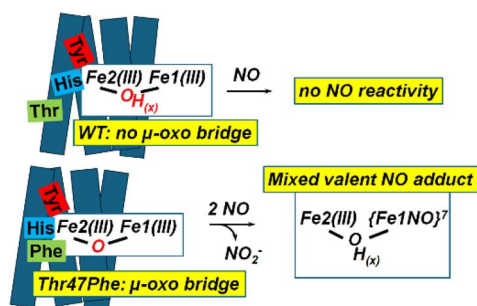
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### A two-dimensional fluorescence and chemiluminescence orthogonal probe for discriminating and quantifying similar proteins

Juan Li, Xiuyan Zhao, Yutao Zhang,\* Yao Lu, Haoyun Xue, Dan Li, Qiang Liu, Chenxu Yan, Weijie Chi, Xingqing Xiao,\* Wei-Hong Zhu and Zhiqian Guo\*

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### A single outer-sphere amino-acid substitution turns on the NO reactivity of a hemerythrin-like protein

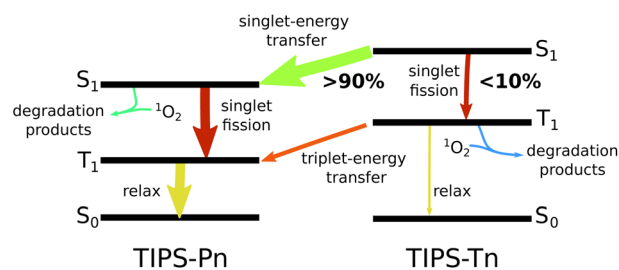
Therese Albert, Natasha Pence, Fangfang Zhong, Ekaterina V. Pletneva and Pierre Moëgne-Loccoz\*



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## Photodegradation reveals that singlet energy transfer impedes energy-gradient-driven singlet fission in polyacene blends

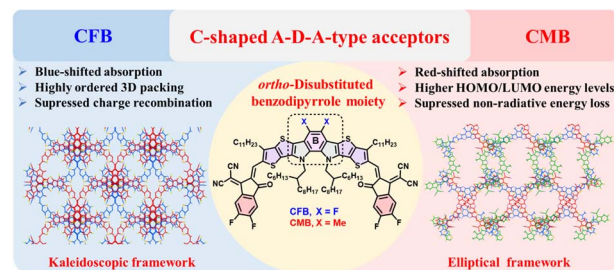
Alexandra N. Stuart,\* Jessica M. de la Perrelle, David M. Huang\* and Tak W. Kee\*



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## Fluorinated and methylated *ortho*-benzodipyrrole-based acceptors suppressing charge recombination and minimizing energy loss in organic photovoltaics

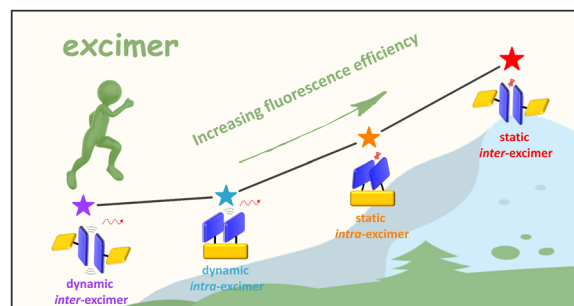
Yan-Bo Wang, Chia-Lin Tsai, Yung-Jing Xue, Bing-Huang Jiang, Han-Cheng Lu, Jun-Cheng Hong, Yu-Chi Huang, Kuo-Hsiu Huang, Su-Ying Chien, Chih-Ping Chen and Yen-Ju Cheng\*



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## A comparative investigation on excimer fluorescence toward its bright future

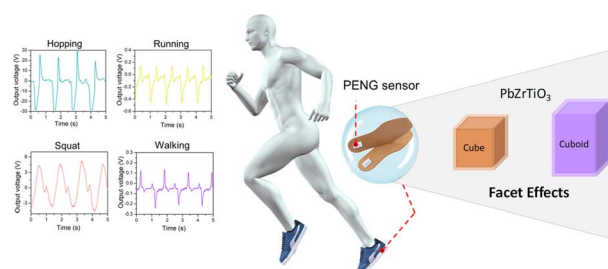
Shiyin Wang, Haichao Liu,\* Shuaiqiang Zhao, Qiaolin Wu, Zhiqiang Yang, Daojie Yang, Yingbo Lv, Qing Su, Shi-Tong Zhang and Bing Yang\*



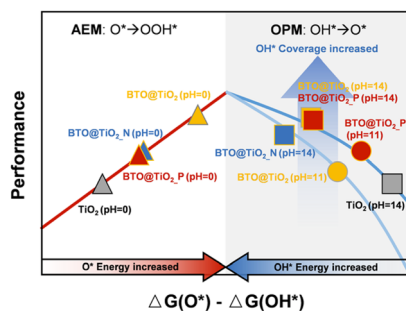
3285

## Synthesis of shape-tunable $\text{PbZrTiO}_3$ nanocrystals with lattice variations for piezoelectric energy harvesting and human motion detection

Ya-Ju Chuang, Arnab Pal, Bo-Hao Chen, Satyaranjan Jena, Sreerag Suresh, Zong-Hong Lin\* and Michael H. Huang\*



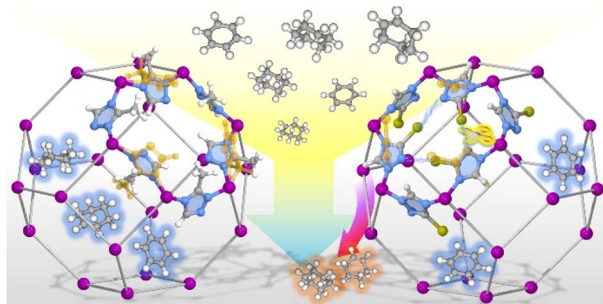
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### Unravelling the pH-dependent mechanism of ferroelectric polarization on different dynamic pathways of photoelectrochemical water oxidation

Xing Ji, Zhouhao Zhu, Ming Zhou, Ying Zhang, Liyong Gan,\* Yunhuai Zhang\* and Peng Xiao\*

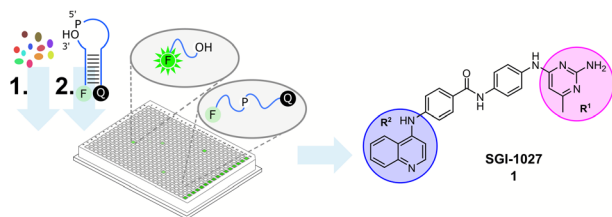
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### Introducing halogen-bonded gates into zeolitic frameworks for efficient benzene/cyclohexene/cyclohexane separation

Zi-Jun Liang, Fang-Di Dong, Le Ye, Kai Zheng, Ding-Yi Hu, Xi Feng, Wen-Yu Su, Zhi-Shuo Wang, Mu-Yang Zhou, Zi-Luo Fang, Dong-Dong Zhou,\* Jie-Peng Zhang\* and Xiao-Ming Chen

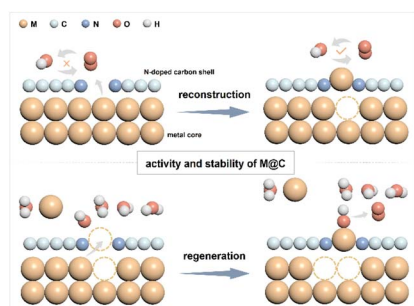
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### Potent inhibitors of the human RNA ligase Rlig1 highlights its role in RNA integrity maintenance under oxidative cellular stress

Lisa A. Schlor, Maya Peußner, Silke Müller and Andreas Marx\*

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### Activity and stability origin of core-shell catalysts: unignorable atomic diffusion behavior

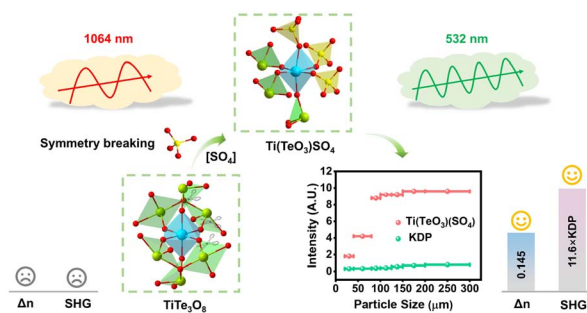
Yuanyuan Xue, Letian Chen, Lijuan Zhang, Gengfeng Zheng,\* Xu Zhang\* and Zhen Zhou\*



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### Different p-block elements induce $C_3[111]$ octahedral distortion in titanium to generate an intense nonlinear effect

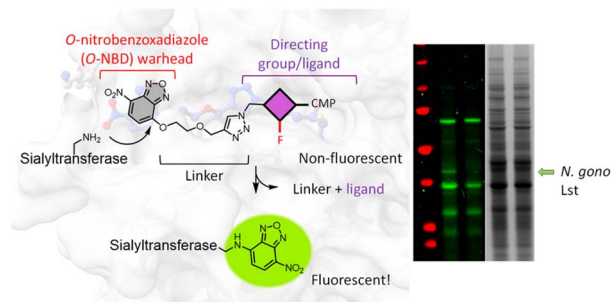
Zhenhua Li, Zhengli Liang, Jiahao Wan, Lehui Liu, Chunxiang Wu, Ping Wang, Xingxing Jiang,\* Zheshuai Lin and Hongming Liu\*



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### Affinity-based covalent sialyltransferase probes enabled by ligand-directed chemistry

Jun Yang Ong, Erianna I. Alvarado-Melendez, Joshua C. L. Maliepaard, Karli R. Reiding and Tom Wennekes\*



## CORRECTION

3345

### Correction: Peptide macrocyclisation via intramolecular interception of visible-light-mediated desulfurisation

Frances R. Smith, Declan Meehan, Rhys C. Griffiths, Harriet J. Knowles, Peiyu Zhang, Huw E. L. Williams, Andrew J. Wilson and Nicholas J. Mitchell\*

