

# Chemical Science

rsc.li/chemical-science

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 16(7) 2937–3348 (2025)



**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.

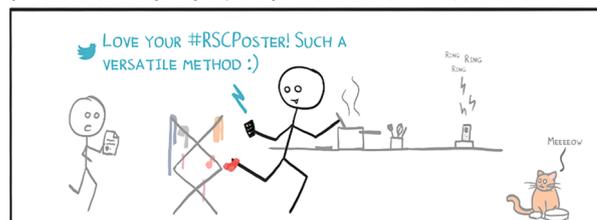
## EDITORIAL

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

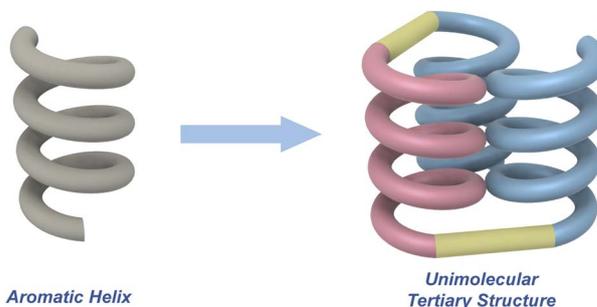
WITH LIVE CARTOONS BY @ERRANTSCIENCE  
MORE INFO AT [RSC.LI/POSTER](https://rsc.li/poster)

## COMMENTARY

2958

### A focus on a complex abiotic tertiary structure

Yulong Zhong and Bing Gong\*



# EES Catalysis

GOLD  
OPEN  
ACCESS

Exceptional research on energy  
and environmental catalysis

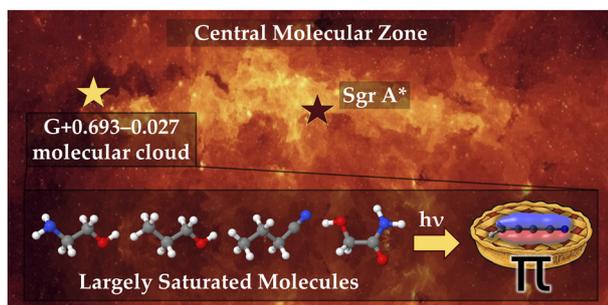
Open to everyone. Impactful for all

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

Fundamental questions  
Elemental answers



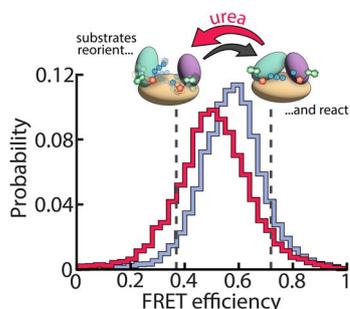
3051



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

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

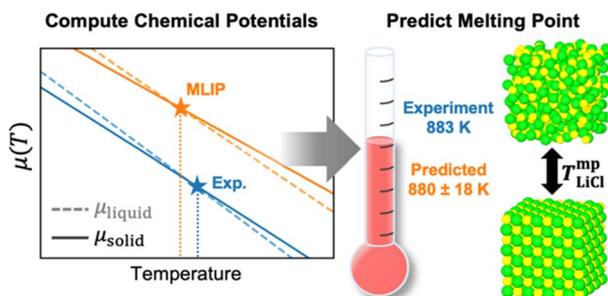
3066



### 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\*

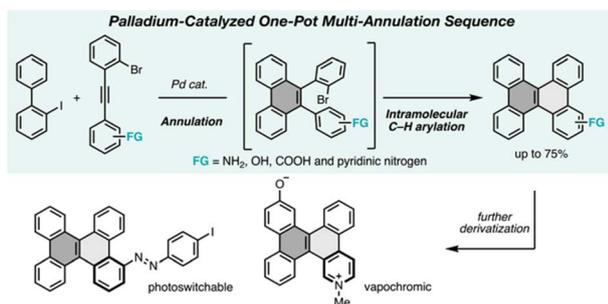
3078



### 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

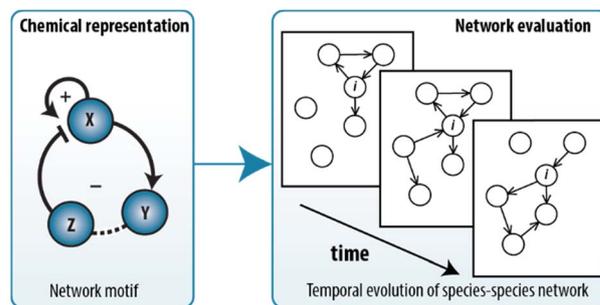
Takehisa Maekawa\* and Kenichiro Itami\*



3099

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

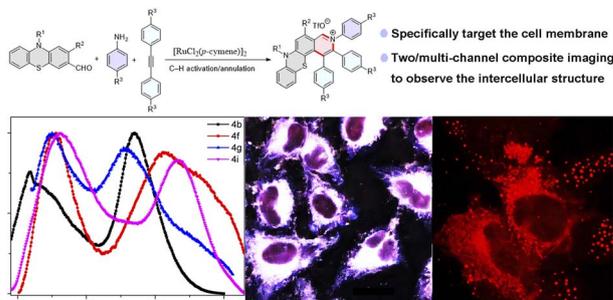
Éverton F. da Cunha, Yanna J. Kraakman, Dmitrii V. Kriukov, Thomas van Poppel, Clara Stegehuis\* and Albert S. Y. Wong\*



3107

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

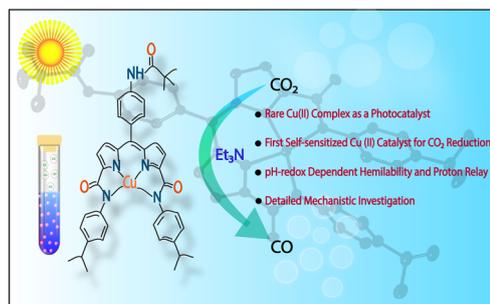
Junxiang Liu, Kangmin Wang, Liqiu Wan, Xianhui Yang and Bijin Li\*



3114

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

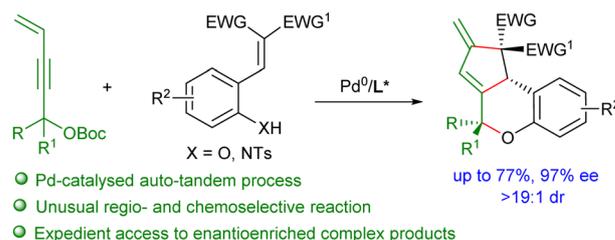
Soumadip Das, Aritra Roy, Navonil Chakrabarti, Narottam Mukhopadhyay, Aniruddha Sarkar and Sayam Sen Gupta\*



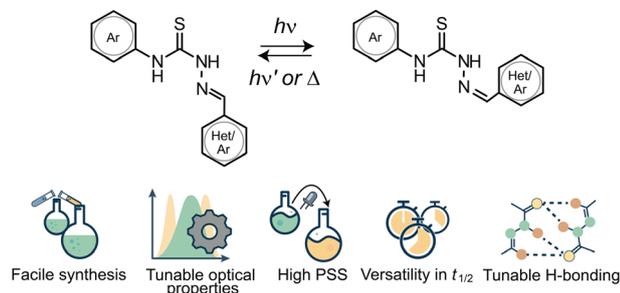
3124

### 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\*



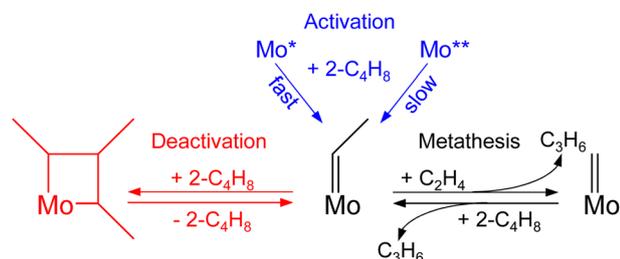
3130



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

Bengi Sentürk, Burkhard Butschke and Fabian Eisenreich\*

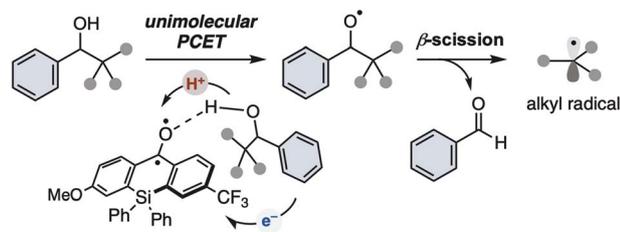
3141



### 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\*

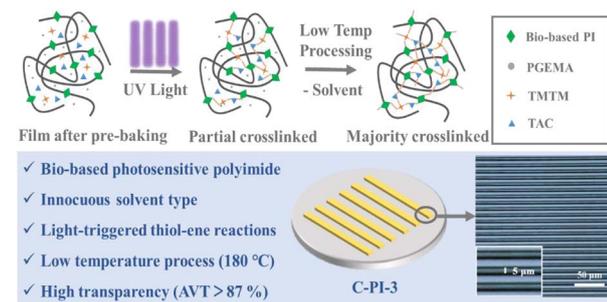
3150



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

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

3157



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

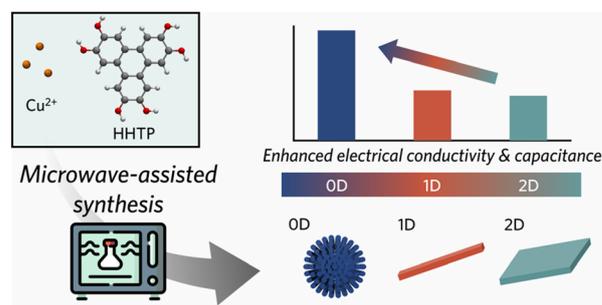
Huifa Meng, Kaijin Chen, Chuying Li, Longfei Zhang, Yanwei He, Zining Zhao, Peixin Wu, Hai Zhu, Zhenguo Chi, Jiarui Xu, Siwei Liu and Yi Zhang\*



3168

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

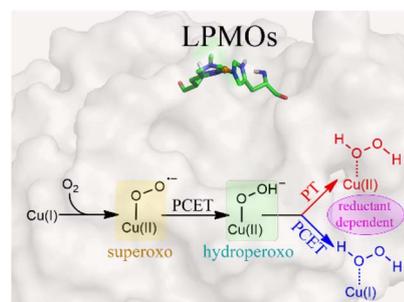
Xiaoyu Fang, Ji Yong Choi, Chenwei Lu, Elizabeth Reichert, Hoai T. B. Pham and Jihye Park\*



3173

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

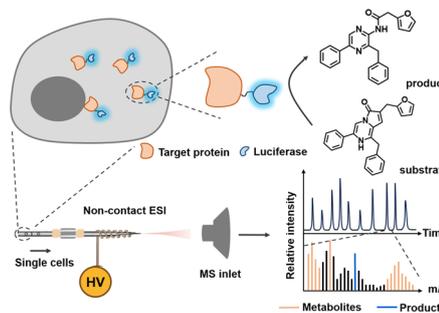
Zhanfeng Wang,\* Xiaodi Fu, Wenwen Diao, Yao Wu,\* Carme Rovira\* and Binju Wang\*



3187

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

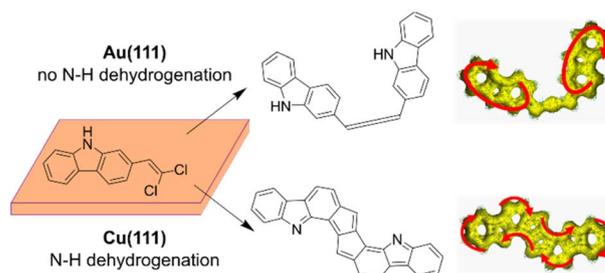
Shaojie Qin, Xinyi Zhang, Yi Zhang, Daiyu Miao, Wensheng Wei and Yu Bai\*



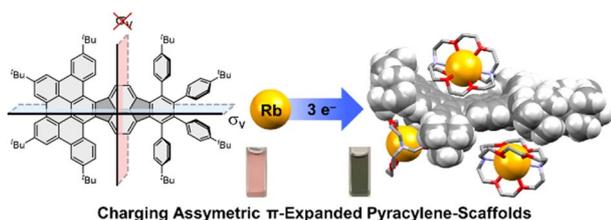
3198

### 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\*



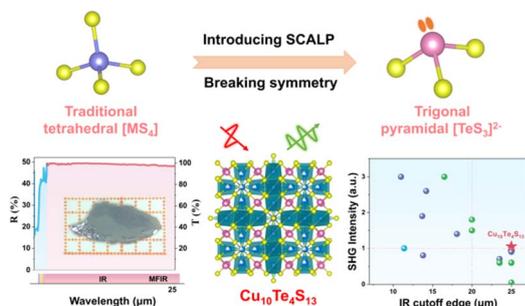
3211



### 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\*

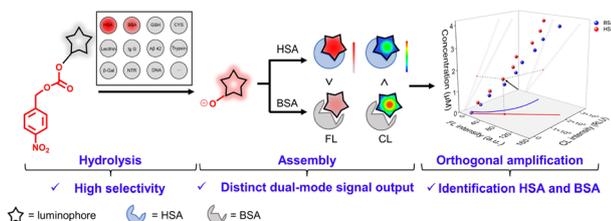
3218



### Exploring new horizons in mid-to-far infrared nonlinear optical crystals: the significant potential of trigonal pyramidal [TeS<sub>3</sub>]<sup>2-</sup> functional units

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

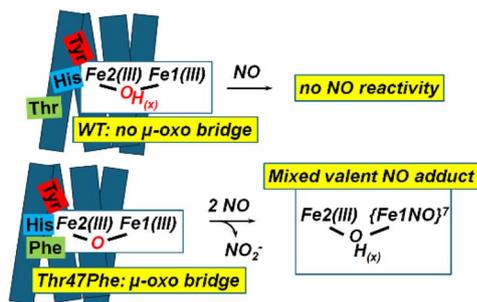
3228



### 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\*

3238



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

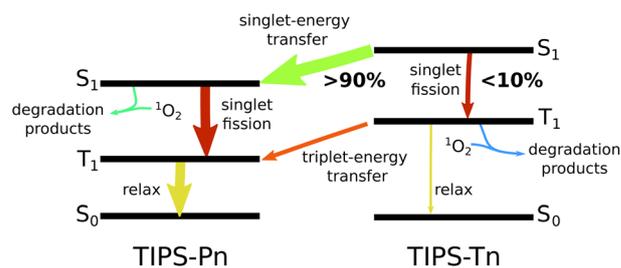
Therese Albert, Natasha Pence, Fangfang Zhong, Ekaterina V. Pletneva and Pierre Moënné-Loccoz\*



3246

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

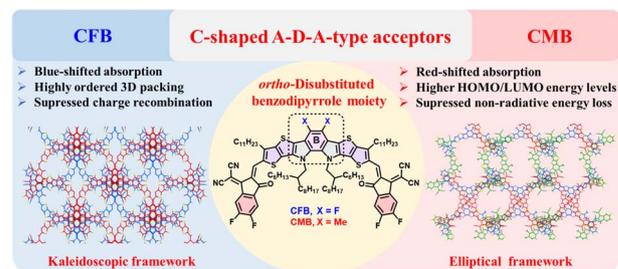
Alexandra N. Stuart,\* Jessica M. de la Perrelle, David M. Huang\* and Tak W. Kee\*



3259

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

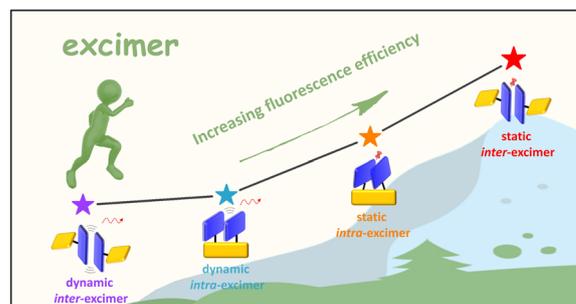
Yan-Bo Wang, Chia-Lin Tsai, Yung-Jing Xue, Bing-Huang Jiang, Han-Cheng Lu, Jun-Cheng Hong, Yu-Chi Huang, Kuo-Hsiu Huang, Su-Ying Chien, Chih-Ping Chen and Yen-Ju Cheng\*



3275

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

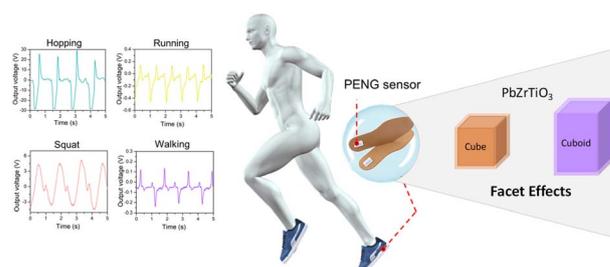
Shiyin Wang, Haichao Liu,\* Shuaiqiang Zhao, Qiaolin Wu, Zhiqiang Yang, Daojie Yang, Yingbo Lv, Qing Su, Shi-Tong Zhang and Bing Yang\*



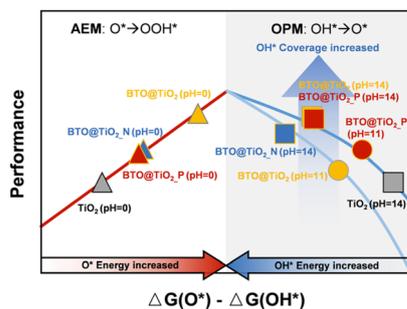
3285

## Synthesis of shape-tunable PbZrTiO<sub>3</sub> 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\*



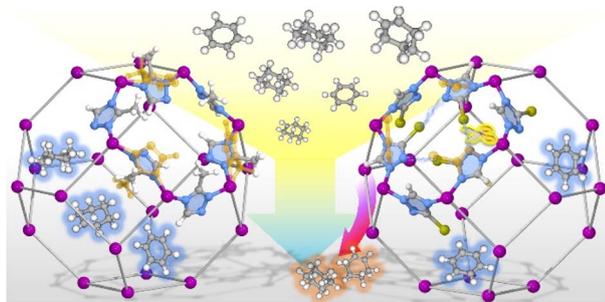
3296



### 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,<sup>\*</sup> Yunhuai Zhang<sup>\*</sup> and Peng Xiao<sup>\*</sup>

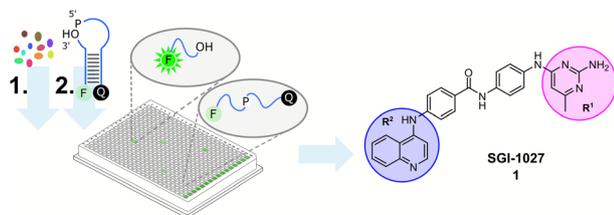
3307



### 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,<sup>\*</sup> Jie-Peng Zhang<sup>\*</sup> and Xiao-Ming Chen

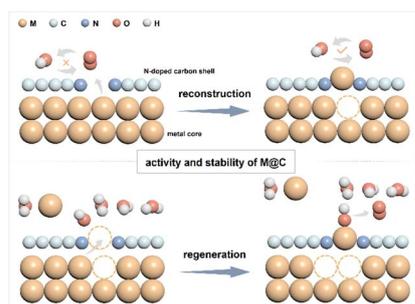
3313



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

3323



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

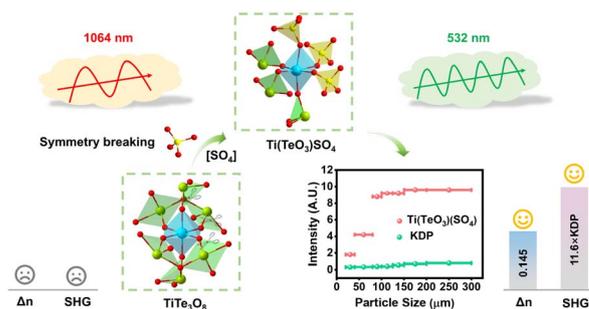
Yuanyuan Xue, Letian Chen, Lijuan Zhang, Gengfeng Zheng,<sup>\*</sup> Xu Zhang<sup>\*</sup> and Zhen Zhou<sup>\*</sup>



3329

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

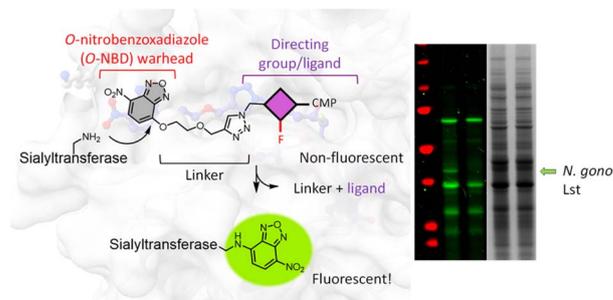
Zhenhua Li, Zhengli Liang, Jiahao Wan, Lehui Liu, Chunxiang Wu, Ping Wang, Xingxing Jiang,\* Zheshuai Lin and Hongming Liu\*



3336

### 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\*

