

# Chemical Science

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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 Heidy 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.

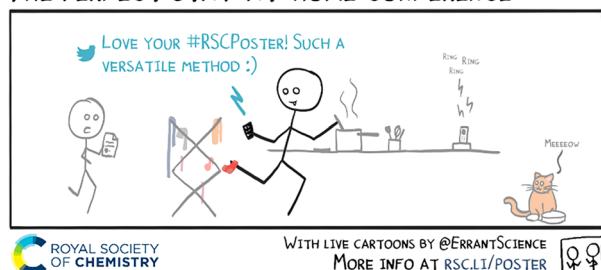
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### Celebrating 10 years of #RSCPoter

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

### THE PERFECT STAY-AT-HOME CONFERENCE

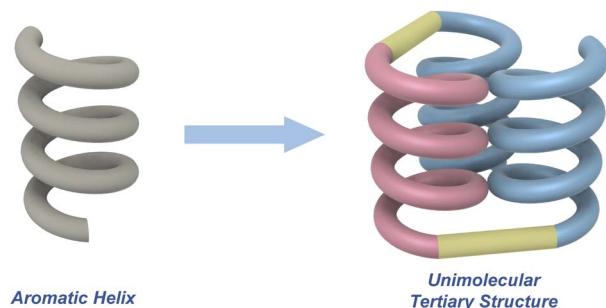


## COMMENTARY

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### A focus on a complex abiotic tertiary structure

Yulong Zhong and Bing Gong\*



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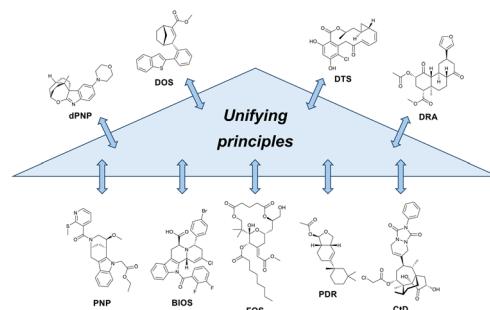
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## PERSPECTIVE

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**Unifying principles for the design and evaluation of natural product-inspired compound collections**

Frederik Simonsen Bro and Luca Laraia\*

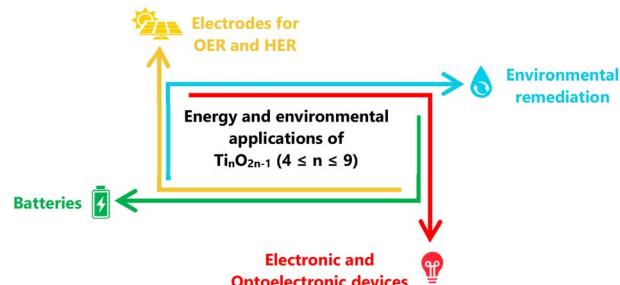


## REVIEWS

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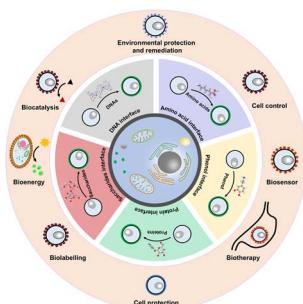
S. Amanda Ekanayake, Haoxin Mai, Dehong Chen and Rachel A. Caruso\*



3019

**Natural biomolecules for cell-interface engineering**

Tong-Kai Zhang, Zi-Qian Yi, Yao-Qi Huang,\* Wei Geng\* and Xiao-Yu Yang\*

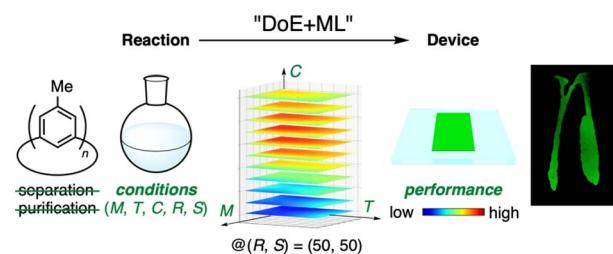


## EDGE ARTICLES

3045

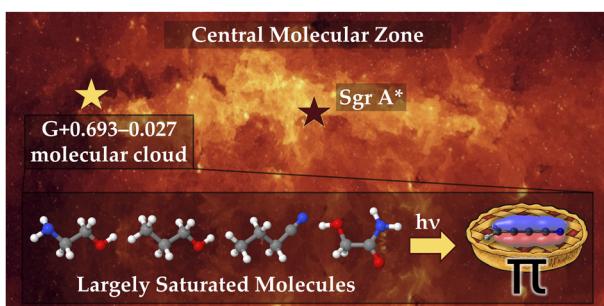
**Optimising reaction conditions in flasks for performances in organic light-emitting devices**

Koki Ikemoto,\* Misato Akiyoshi, Ayano Kobayashi, Hiroshi Kita, Hideo Taka and Hiroyuki Isobe\*



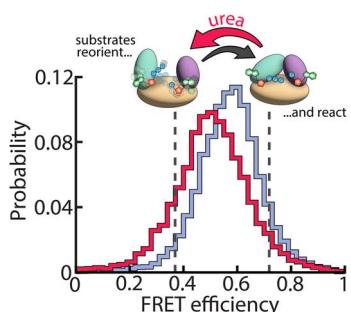
## EDGE ARTICLES

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

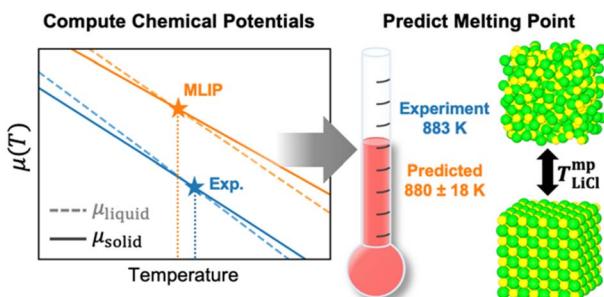
Jhoan Londoño-Restrepo, Santiago Gómez, Heidy M. Quitián-Lara,\* Felipe Fantuzzi\* and Albeiro Restrepo\*

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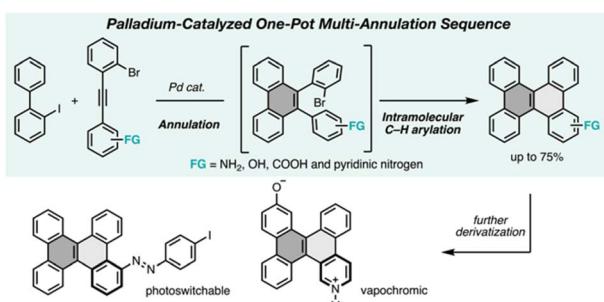
David Scheerer,\* Dorit Levy, Remi Casier, Inbal Riven, Hisham Mazal and Gilad Haran\*

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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\*

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

Takehisa Maekawa\* and Kenichiro Itami\*

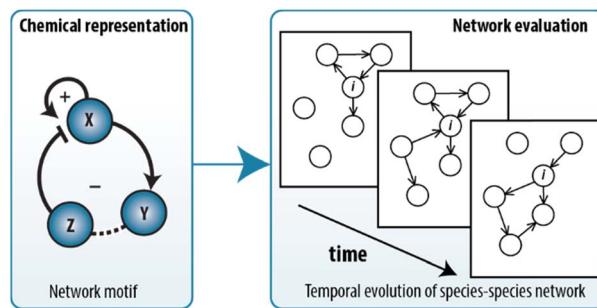


## EDGE ARTICLES

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

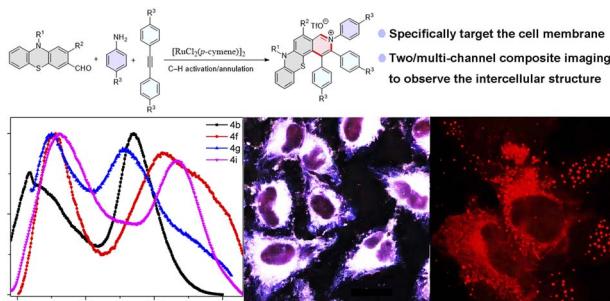
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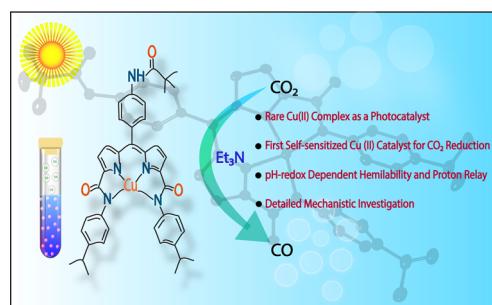
Junxiang Liu, Kangmin Wang, Ligu Wan, Xianhui Yang and Bijin Li\*



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**Self-sensitized Cu(II)-complex catalyzed solar driven  $\text{CO}_2$  reduction**

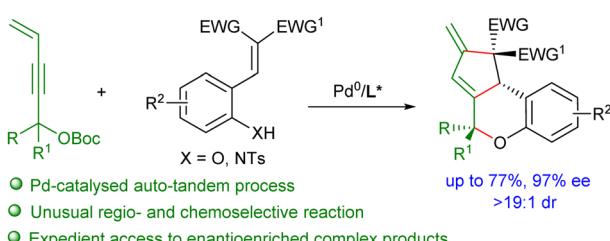
Soumadip Das, Aritra Roy, Navonil Chakrabarti, Narottam Mukhopadhyay, Aniruddha Sarkar and Sayam Sen Gupta\*



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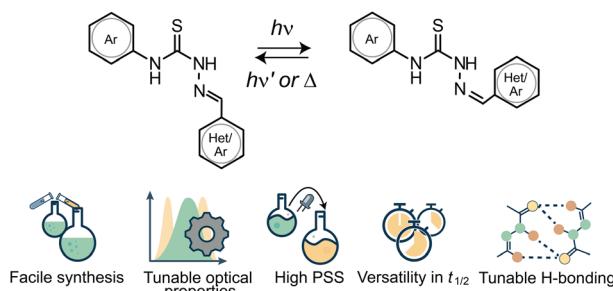
**Palladium-catalysed asymmetric cascade transformations of 4-alken-2-ynyl carbonates to construct complex frameworks**

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



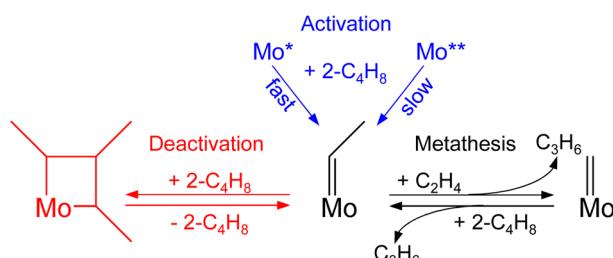
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**Thiosemicarbazones as versatile photoswitches with light-controllable supramolecular activity**

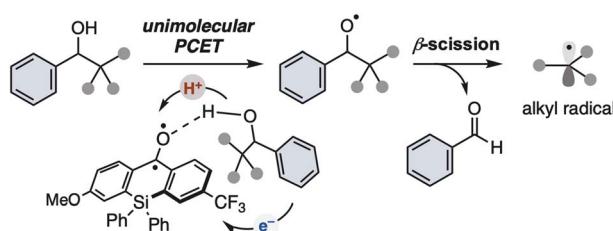
Bengi Sentürk, Burkhard Butschke and Fabian Eisenreich\*

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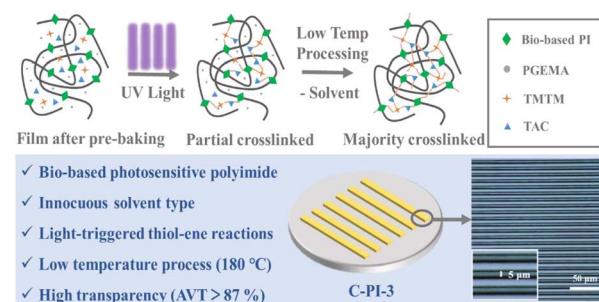
Tatiana Otroshchenko,\* Aleksandr Fedorov, Qiyang Zhang, David Linke, Jarosław Handzlik, Mirjam Schröder, Björn Corzilius and Evgenii V. Kondratenko\*

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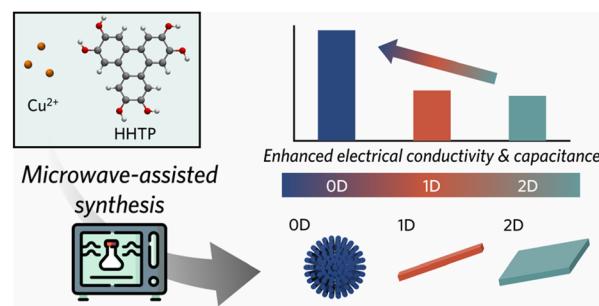
**Innocuous solvent-based, low-temperature curable, and highly transparent photosensitive polyimides developed using soluble polyimides containing bio-based magnolol moieties**

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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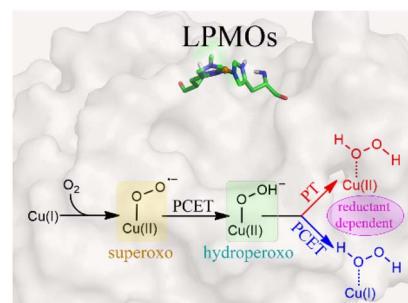
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**From 0D to 2D: microwave-assisted synthesis of electrically conductive metal–organic frameworks with controlled morphologies**Xiaoyu Fang, Ji Yong Choi, Chenwei Lu,  
Elizabeth Reichert, Hoai T. B. Pham and Jihye Park\*

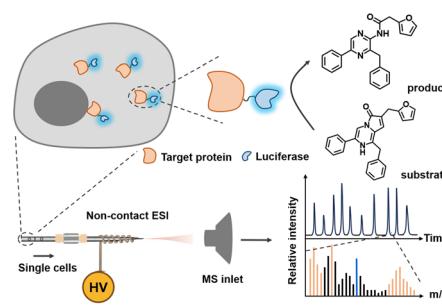
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**Theoretical study of the *in situ* formation of H<sub>2</sub>O<sub>2</sub> by lytic polysaccharide monooxygenases: the reaction mechanism depends on the type of reductant**

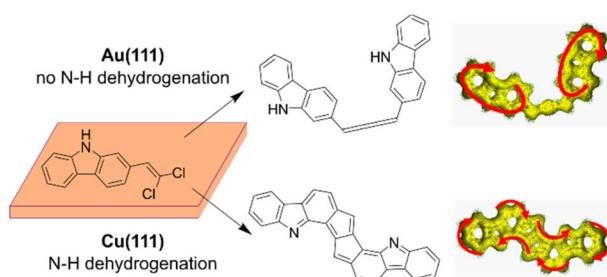
Zhanfeng Wang,\* Xiaodi Fu, Wenwen Diao, Yao Wu,\* Carme Rovira\* and Binju Wang\*



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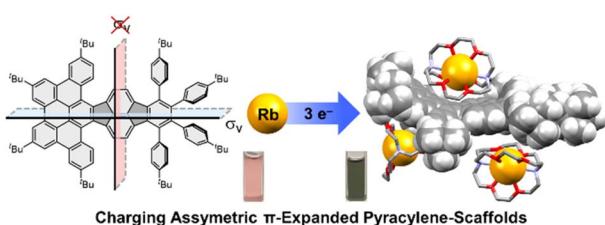
**Multi-dimensional bio mass cytometry: simultaneous analysis of cytoplasmic proteins and metabolites on single cells**Shaojie Qin, Xinyi Zhang, Yi Zhang, Daiyu Miao,  
Wensheng Wei and Yu Bai\*

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Christian Loppacher, Federica Bondino, Elena Magnano,  
Hiroshi Imada, Emiko Kazuma, Yousoo Kim,  
Luca Giovanelli\* and Sylvain Clair\*

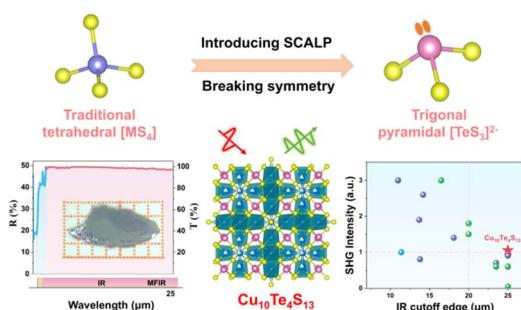
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**Stepwise reduction of an asymmetric  $\pi$ -expanded pyracylene towards the crystalline radical trianion**

Yikun Zhu, Jan Borstelmann, Christian Neiss, Zheng Wei, Andreas Görling, 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  $[\text{TeS}_3]^{2-}$  functional units**

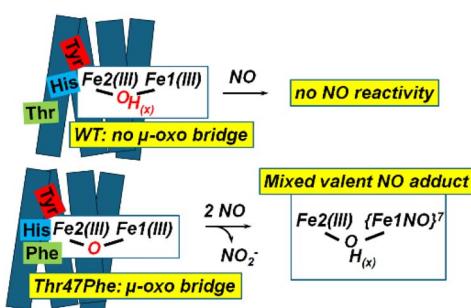
Bo Zhang, Sheng-Hua Zhou,\* Bing-Xuan Li, Xin-Tao Wu, Hua Lin\* and Qi-Long Zhu\*

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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 Moënne-Loccoz\*

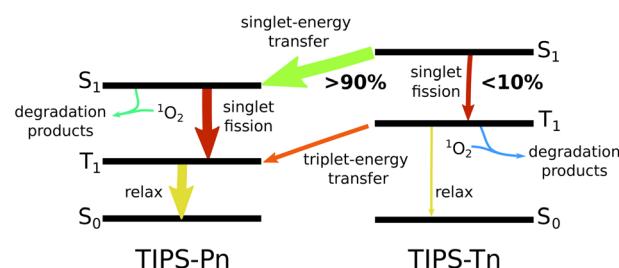


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**Photodegradation reveals that singlet energy transfer impedes energy-gradient-driven singlet fission in polyacene blends**

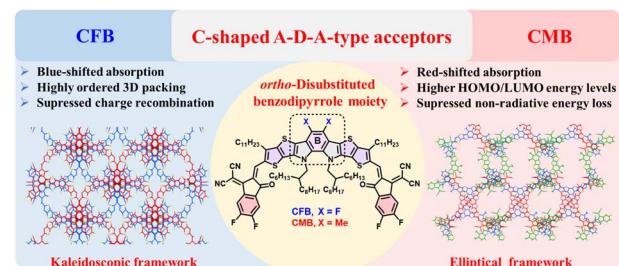
Alexandra N. Stuart,\* Jessica M. de la Perrelle, David M. Huang\* and Tak W. Kee\*



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

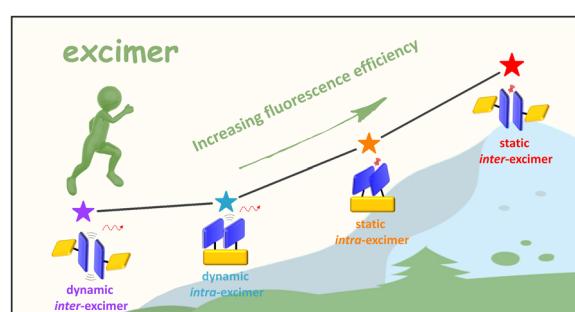
Yan-Bo Wang, Chia-Lin Tsai, Yung-Jing Xue, Bing-Huang Jiang, Han-Cheng Lu, Jun-Cheng Hong, Yu-Chi Huang, Kuo-Hsiu Huang, Su-Ying Chien, Chih-Ping Chen and Yen-Ju Cheng\*



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

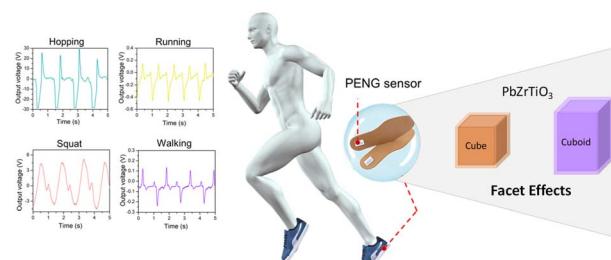
Shiyin Wang, Haichao Liu,\* Shuaiqiang Zhao, Qiaolin Wu, Zhiqiang Yang, Daojie Yang, Yingbo Lv, Qing Su, Shi-Tong Zhang and Bing Yang\*



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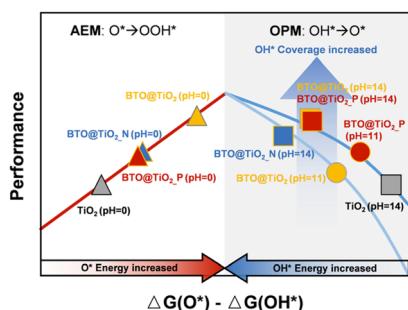
**Synthesis of shape-tunable PbZrTiO<sub>3</sub> nanocrystals with lattice variations for piezoelectric energy harvesting and human motion detection**

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



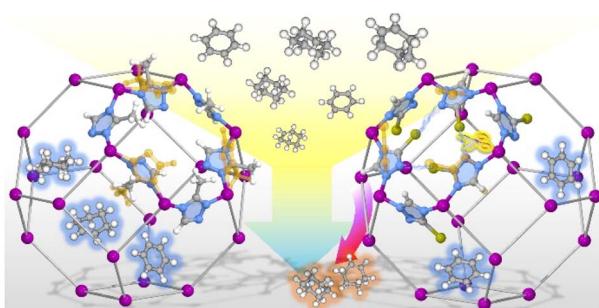
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**Unravelling the pH-dependent mechanism of ferroelectric polarization on different dynamic pathways of photoelectrochemical water oxidation**

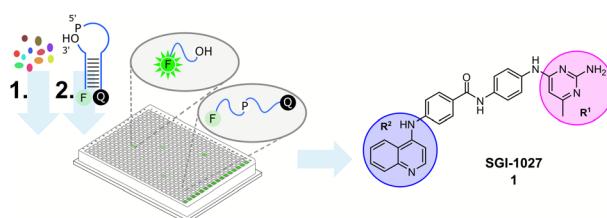
Xing Ji, Zhouhao Zhu, Ming Zhou, Ying Zhang, Liyong Gan,\* Yunhuai Zhang\* and Peng Xiao\*

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**Introducing halogen-bonded gates into zeolithic frameworks for efficient benzene/cyclohexene/cyclohexane separation**

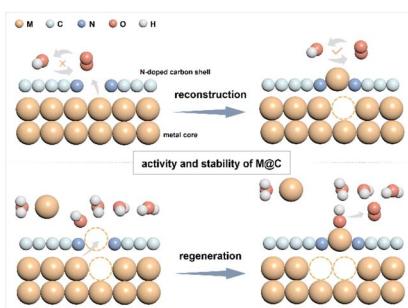
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**Potent inhibitors of the human RNA ligase Rlgl1 highlights its role in RNA integrity maintenance under oxidative cellular stress**

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\*

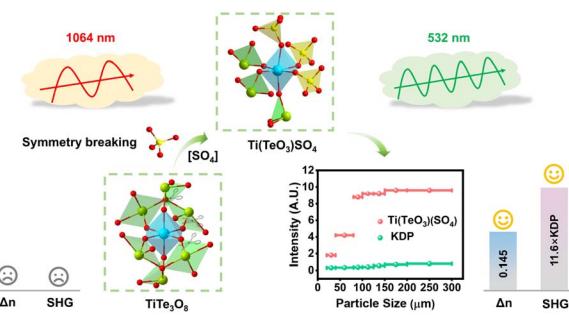


## EDGE ARTICLES

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**Different p-block elements induce C<sub>3</sub>[111] octahedral distortion in titanium to generate an intense nonlinear effect**

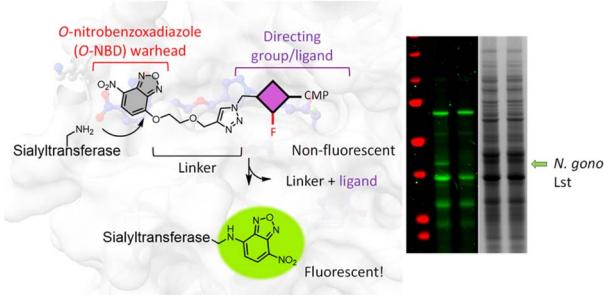
Zhenhua Li, Zhengli Liang, Jiahao Wan, Lehui Liu, Chunxiang Wu, Ping Wang, Xingxing Jiang,\* Zheshuai Lin and Hongming Liu\*



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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\*

