

# Chemical Science

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### Cover

See Zheng Zhou and Marina A. Petrukhina, pp. 468–479.  
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### Inside cover

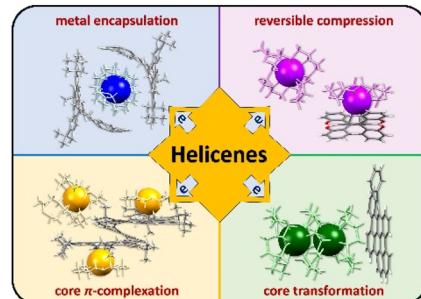
See Renana Gershoni-Poranne et al., pp. 575–583.  
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Image created by Dr. Vitalii Stetsovych.

## PERSPECTIVES

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### Adding multiple electrons to helicenes: how they respond?

Zheng Zhou and Marina A. Petrukhina\*



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### Best-of-both-worlds computational approaches to difficult-to-model dissociation reactions on metal surfaces

Geert-Jan Kroes\* and Jörg Meyer

- Appropriate non-adiabatic dynamics
  - Adjustable hybrid functionals
  - First-principles-based barriers
- Chemical accuracy for dissociative chemisorption on metal surfaces



# EES Batteries

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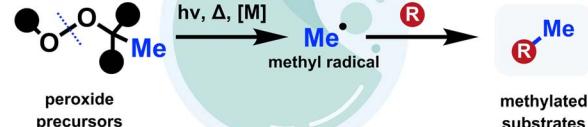
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## REVIEWS

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**Magic methylation with methyl-containing peroxides**

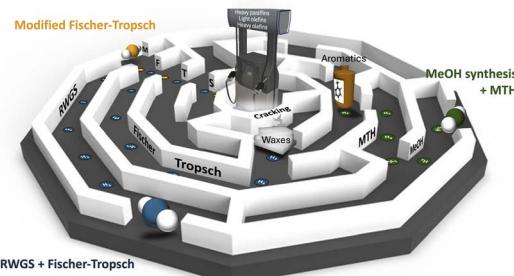
Daliah Farajat, Yuhua Zhang and Chao-Jun Li\*

**Magic Methylation with Methyl-Containing Peroxides**

530

**Potential pathways for CO<sub>2</sub> utilization in sustainable aviation fuel synthesis**

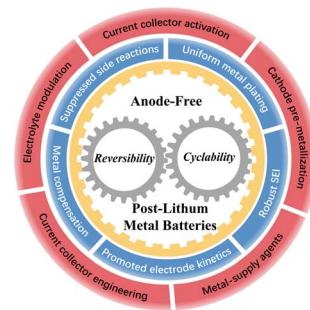
Enrique V. Ramos-Fernandez, Jose L. Santos, Dina K. Alsaadi, Anastasiya Bavykina, Jean Marcel R. Gallo and Jorge Gascon\*



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**The challenges and strategies towards high-performance anode-free post-lithium metal batteries**

Jiawei Wang, Yaosong Zhou, Yanyi Zhuo, Kun Fang, Sicong Wang, Bin Zhao,\* Jing Zhou\* and Hua Wang\*

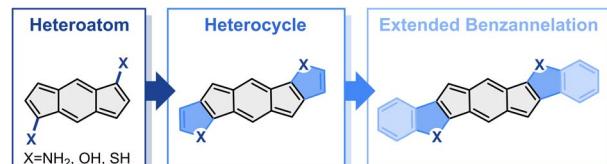


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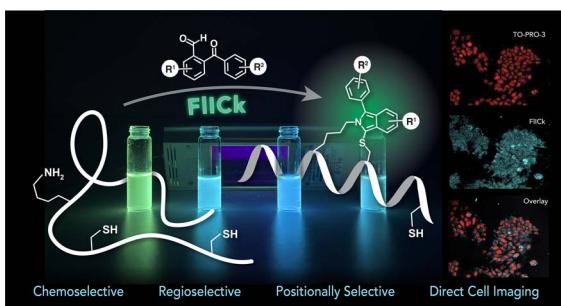
**Effects of benzoheterocyclic annelation on the s-indacene core: a computational analysis**

Gabrielle I. Warren, Katarzyna Młodzikowska-Pieńko, Said Jalife, Isabella S. Demachkie, Judy I. Wu, Michael M. Haley and Renana Gershoni-Poranne\*



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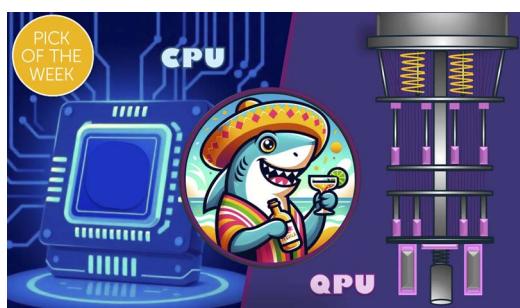
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**Chemoselective, regioselective, and positionally selective fluorogenic stapling of unprotected peptides for cellular uptake and direct cell imaging**

Naysilla L. Dayanara, Juliette Froelich, Pascale Roome and David M. Perrin\*

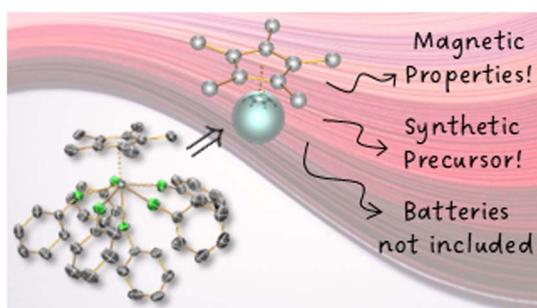
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**SHARC meets TEQUILA: mixed quantum-classical dynamics on a quantum computer using a hybrid quantum-classical algorithm**

Eduarda Sangiogo Gil,\* Markus Oppel, Jakob S. Kottmann and Leticia González\*

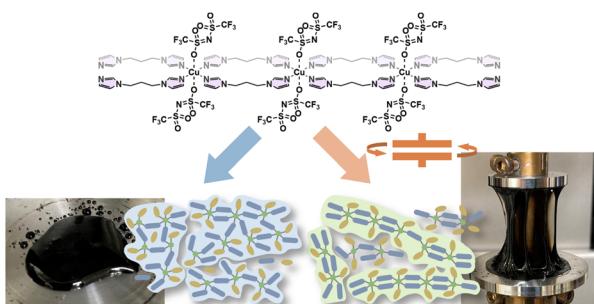
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**A fluorobenzene-bound dysprosium half-sandwich dication single-molecule magnet**

Sophie C. Corner, William J. A. Blackmore, Gemma K. Gransbury, Andrea Mattioni, George F. S. Whitehead, Nicholas F. Chilton\* and David P. Mills\*

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**Mechanically induced polyamorphism in a one-dimensional coordination polymer**

Taichi Nishiguchi, Yuki Ohara, Kentaro Kadota, Xin Zheng, Shin-ichiro Noro and Satoshi Horike\*

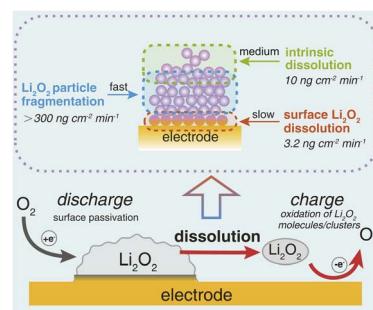


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**Sluggish  $\text{Li}_2\text{O}_2$  dissolution – a key to unlock high-capacity lithium–oxygen batteries**

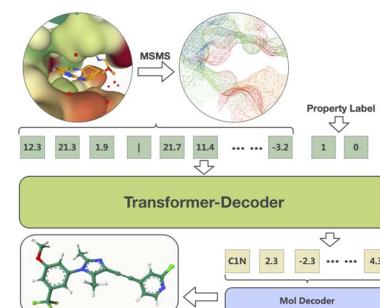
Lu He, Shuo Wang, Fengjiao Yu and Yuhui Chen\*



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**3DSMILES-GPT: 3D molecular pocket-based generation with token-only large language model**

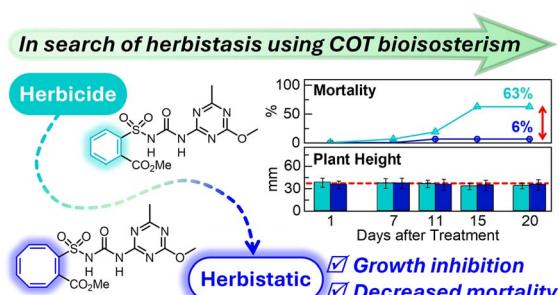
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**In search of herbistasis: COT-metsulfuron methyl displays rare herbistatic properties**

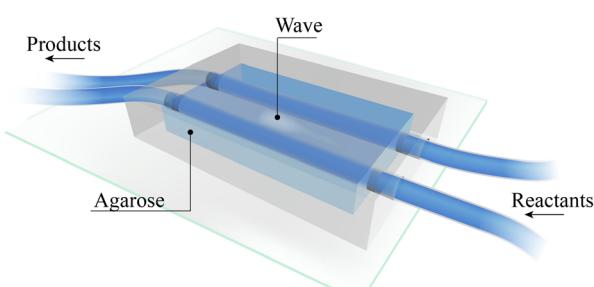
Hui Xing, Sarah K. M. McGregor, Bruna D. Batista, Cassidy Whitefield, Isobella S. J. Stone, Cody-Ellen Murray, Rebecca M. Hurst, Yizhou Liu, Sharon Chow, Tyler Fahrenhorst-Jones, Qi Zhao, Sevan D. Houston, Shu-Hong Hu, Thierry Lohnienne, Amanda Nouwens, Jed M. Burns, G. Paul Savage, Gimme H. Walter, Luke W. Guddat, Michelle A. Rafter and Craig M. Williams\*



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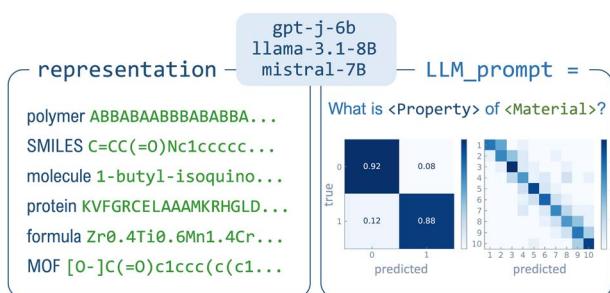
**Chemical waves in reaction-diffusion networks of small organic molecules**

Arpita Paikar, Xiuxiu Li, Liat Avram, Barbara S. Smith, István Sütő, Dezső Horváth, Elisabeth Rennert, Yuqing Qiu, Ágota Tóth, Suriyanarayanan Vaikuntanathan and Sergey N. Semenov\*



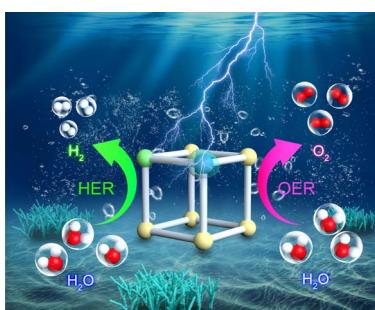
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**Assessment of fine-tuned large language models for real-world chemistry and material science applications**

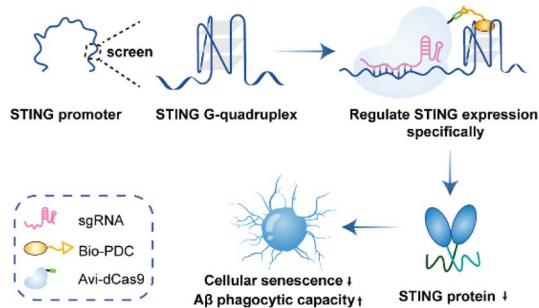
Joren Van Herck et al.

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**Rare-earth element doped NiFe-MOFs as efficient and robust bifunctional electrocatalysts for both alkaline freshwater and seawater splitting**

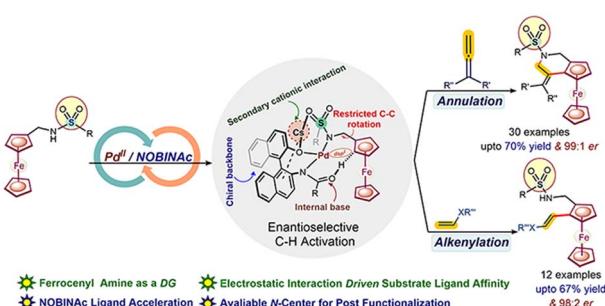
Jun Yang, Yong Shen, Jiahui Xian, Runan Xiang and Guangqin Li\*

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**Regulation of STING G-quadruplex for rescuing cellular senescence and Aβ phagocytic capacity of microglia**

Heying Yuan, Jie Yang, Geng Qin, Yue Sun, Chuanqi Zhao, Chunyu Wang, Jinsong Ren and Xiaogang Qu\*

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**Substrate NOBINAc ligand affinity for Pd<sup>II</sup>-catalyzed enantioselective C–H activation over reactive β-C–H bonds in ferrocenyl amines**

Devendra Parganiha, Raviraj Ananda Thorat, Ashwini Dilip Dhumale, Yagya Dutt Upadhyay, Raushan Kumar Jha, Saravanan Raju and Sangit Kumar\*

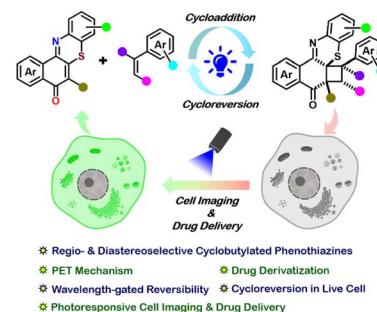


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**Regio- and diastereoselective synthesis of cyclobutylated phenothiazines via [2 + 2] photocycloaddition: demonstrating wavelength-gated cycloreversion inside live cells**

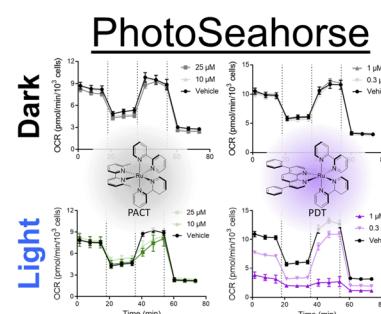
Sanhati Sharangi, Barsha Chakraborty, Raushan Kumar Jha, Swarnadeep Mandal, Apurba Lal Koner\* and Sangit Kumar\*



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**Photodynamic therapy photosensitzers and photoactivated chemotherapeutics exhibit distinct bioenergetic profiles to impact ATP metabolism**

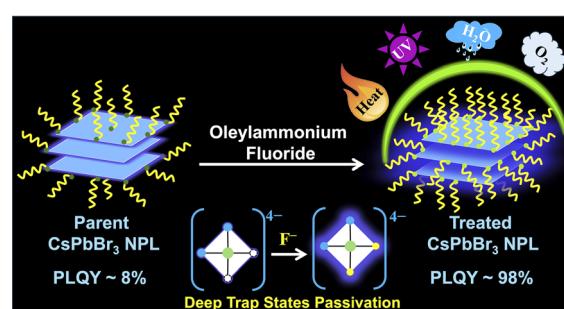
Richard J. Mitchell, Dmytro Havrylyuk, Austin C. Hachey, David K. Heidary\* and Edith C. Glazer\*



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**Oleylammonium fluoride passivated blue-emitting 2D CsPbBr<sub>3</sub> nanoplates with near-unity photoluminescence quantum yield: safeguarding against threats from external perturbations**

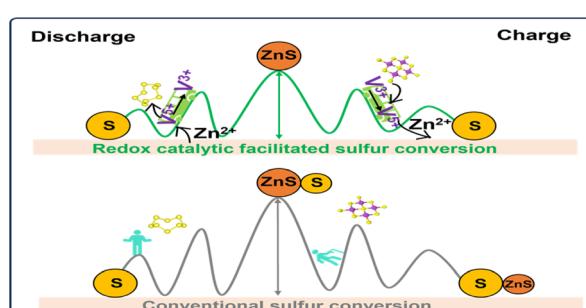
Arghya Sen, Abhijit Dutta, Abir Lal Bose and Pratik Sen\*



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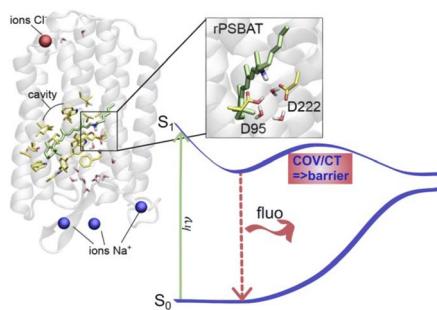
**Reconstructing the phase of vanadium oxides enables redox-catalysis manipulated reversible sulfur conversion for stable Zn–S batteries**

Hao Luo,\* Fan Li, Mingli Wang,\* Shang Sun, Min Zhou, Wenjing Zhang, Hengrui Guo, Xueyin Su, Xiaolong Li\* and Lina Ma\*



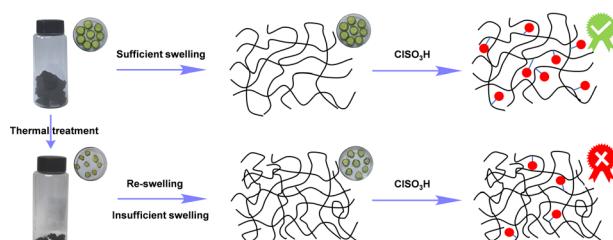
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**Archaerhodopsin 3 is an ideal template for the engineering of highly fluorescent optogenetic reporters**

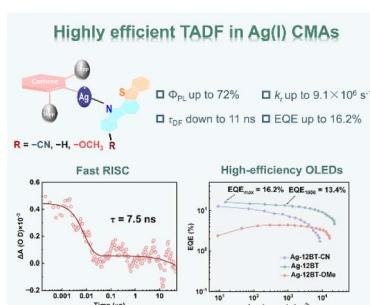
Krystyna Herasymenko, Danushka Walisinghe, Masaë Konno, Leonardo Barneschi, Isabelle de Waele, Michel Sliwa, Keiichi Inoue,\* Massimo Olivucci\* and Stefan Haacke\*

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**Efficient construction of high-quality sulfonated porous aromatic frameworks by optimizing the swelling state of porous structures**

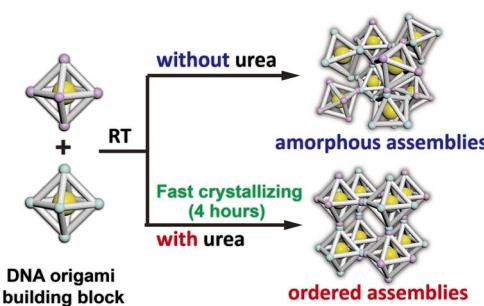
Lulu Yang, Zhen Zhan, Lin Zhao, Chengxin Zhang, Shaolei Wang,\* Wei Hu\* and Guangshan Zhu\*

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**Ag(I) emitters with ultrafast spin-flip dynamics for high-efficiency electroluminescence**

Ao Ying, Nengquan Li, Xingyu Chen, Jianlong Xia, Chuluo Yang\* and Shaolong Gong\*

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**Fast synthesis of DNA origami single crystals at room temperature**

Yifan Yu, Min Ji, Yong Wang, Xuehui Yan, Lizhi Dai, Ningning Ma, Zhaoyu Zhou, Hang Xing and Ye Tian\*

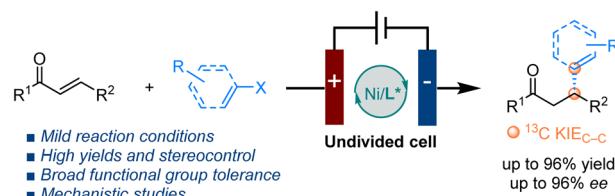


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**Enantioselective nickel-catalyzed electrochemical reductive conjugate alkenylation of  $\alpha,\beta$ -unsaturated ketones**

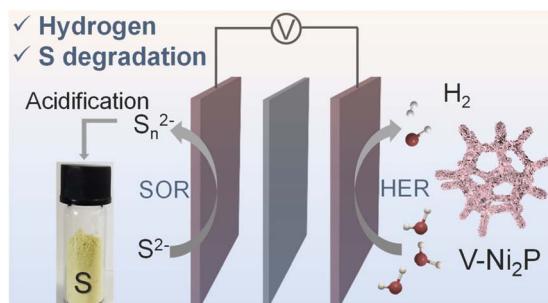
Siriphong Somprasong,\* Bin Wan and Syuzanna R. Harutyunyan\*



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**Vanadium-regulated nickel phosphide nanosheets for electrocatalytic sulfion upgrading and hydrogen production**

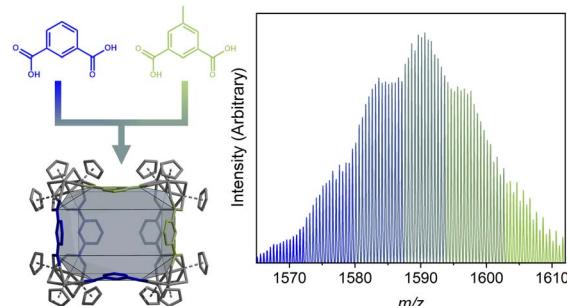
Rui-Qing Li,\* Xiaojun Wang, Shuxiang Xie, Songyun Guo, Zhe Cao, Zhenhao Yan, Wei Zhang\* and Xiaoyu Wan\*



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**Tunable synthesis of heteroleptic zirconium-based porous coordination cages**

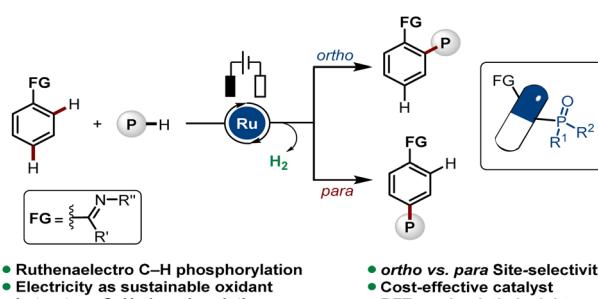
Merissa N. Morey, Christine M. Montone, Michael R. Dworzak, Glenn P. A. Yap and Eric D. Bloch\*



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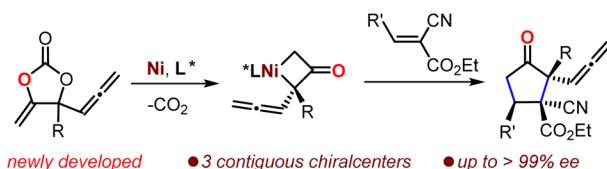
**Ruthenaelectro-catalyzed C–H phosphorylation: *ortho* to *para* position-selectivity switch**

Xue-Ya Gou, João C. A. Oliveira, Shan Chen, Simon L. Homölle, Sven Trienes, Tristan von Münchow, Bo-Sheng Zhang and Lutz Ackermann\*



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**Ni-catalyzed asymmetric decarboxylation for the construction of carbocycles with contiguous quaternary carbon stereocenters**

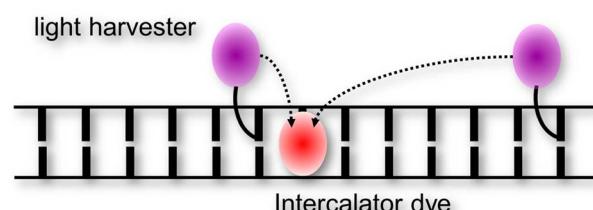
Yicheng He, Biwei Yan, Cheng Ma, Shaofei Ni and Wusheng Guo\*

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**Tetrapodal iron complexes invoke observable intermediates in nitrate and nitrite reduction**

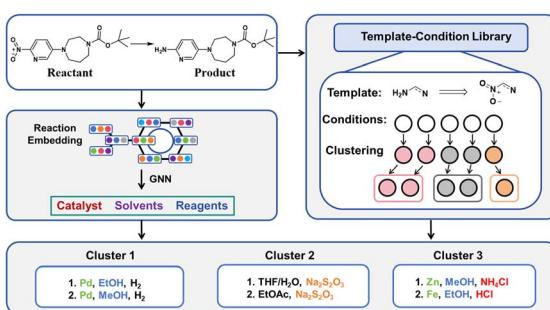
Jewelianna M. Moore and Alison R. Fout\*

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**Light harvesting FIT DNA hybridization probes for brightness-enhanced RNA detection**

Amal Homer, Andrea Knoll, Uschi Gruber and Oliver Seitz\*

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**Reacon: a template- and cluster-based framework for reaction condition prediction**

Zihan Wang, Kangjie Lin, Jianfeng Pei\* and Luhua Lai\*

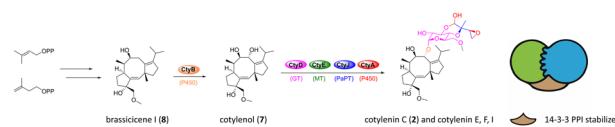


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**Total biosynthesis of cotylenin diterpene glycosides as 14-3-3 protein–protein interaction stabilizers**

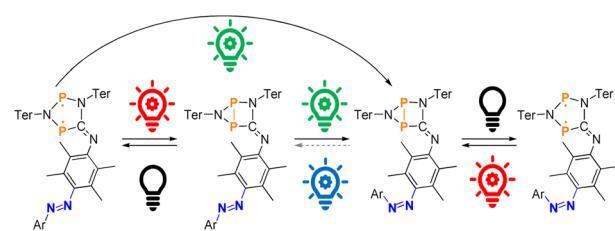
Zhenhua Guan, Nanyu Yao, Wenling Yuan, Fengli Li, Yang Xiao, Mewlude Rehmutulla, Yuhua Xie, Chunmei Chen, Hucheng Zhu, Yuan Zhou, Qingyi Tong, Zheng Xiang,\* Ying Ye\* and Yonghui Zhang\*



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**Designing a visible light-mediated double photoswitch: a combination of biradical and azobenzene structural motifs that can be switched independently**

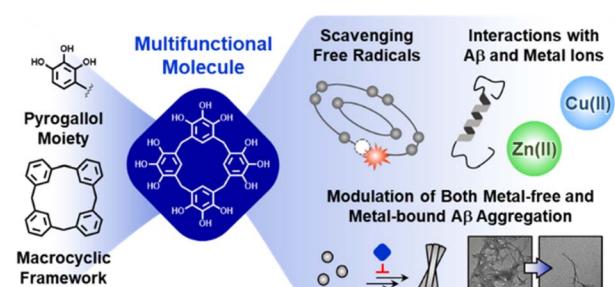
Yannic Pilopp, Henrik Beer, Jonas Bresien, Dirk Michalik, Alexander Villinger and Axel Schulz\*



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**Multi-target macrocycles: pyrogallol derivatives to control multiple pathological factors associated with Alzheimer's disease**

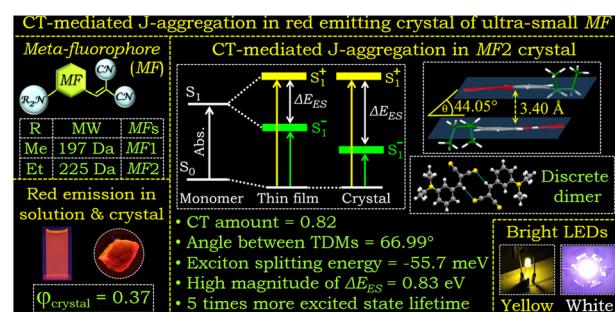
Jimin Kwak, Yelim Yi, Seongmin Park and Mi Hee Lim\*



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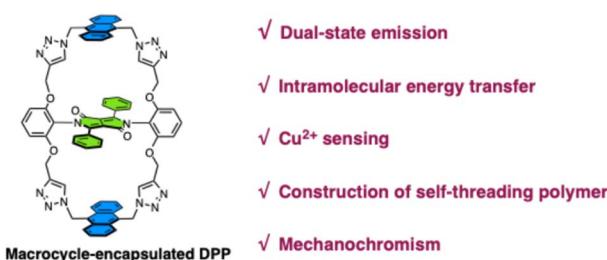
**Charge-transfer mediated J-aggregation in red emitting ultra-small-single-benzenic meta-fluorophore crystals**

Mrinal Mandal, Sukumar Mardanya, Arjit Saha, Manjeet Singh, Swarnali Ghosh, Tanmay Chatterjee, Ramen Patra, Surojit Bhunia, Saptarshi Mandal, Soumen Mukherjee, Rahul Debnath, C. Malla Reddy, Mousumi Das and Prasun K. Mandal\*



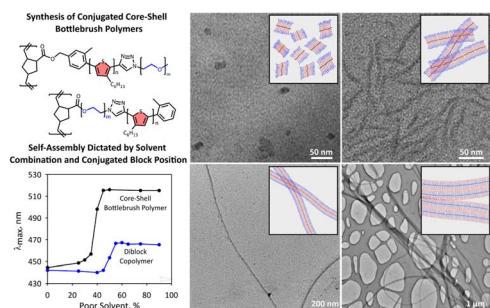
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**Internally diketopyrrolopyrrole-bridged bis-anthracene macrocycle: a multifunctional fluorescent platform**

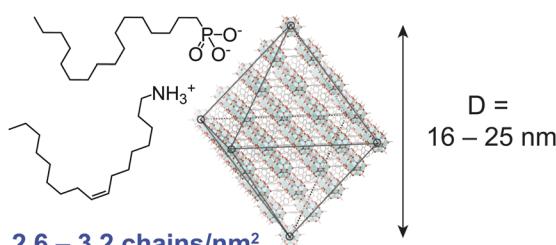
Huan Zhou, Yuxuan Zhang, Zhiye Zheng, Junhua Wan,\* Hui Zhang, Kunhua Lin,\* Jonathan L. Sessler\* and Hongyu Wang\*

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**Conjugated core–shell bottlebrush polymers that exhibit crystallization-driven self-assembly**

Victor Lotocki, Alicia M. Battaglia, Nahye Moon, Hatem M. Titi and Dwight S. Seferos\*

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*Sterically Stabilized MOF Nanocrystal Colloids*

**Steric stabilization of colloidal UiO-66 nanocrystals with oleylammonium octadecylphosphonate**

Sungho V. Park, Lakshmi Bhai, Gahyun Annie Lee, Ah-Hyung Alissa Park, Lauren E. Marbella and Jonathan S. Owen\*

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**Lattice oxygen insertion mechanism in CeO<sub>2</sub>-catalyzed reactions in water: nitrile hydration reaction**

Takaaki Endo, Tatsushi Ikeda, Koki Muraoka, Yusuke Kita, Masazumi Tamura\* and Akira Nakayama\*

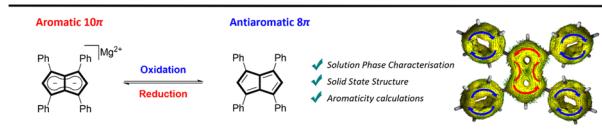


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**Reversible formation of tetraphenylpentalene, a room temperature stable antiaromatic hydrocarbon**

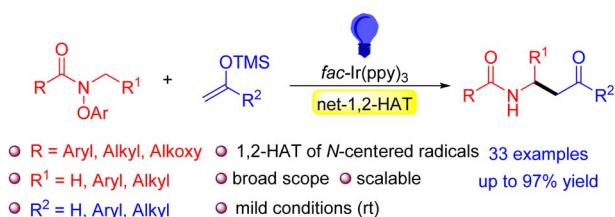
Hugh J. Sanderson, Andreas Helbig,  
Gabriele Kociok-Köhn, Holger Helten\*  
and Ulrich Hintermair\*



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**Visible-light-driven net-1,2-hydrogen atom transfer of amidyl radicals to access  $\beta$ -amido ketone derivatives**

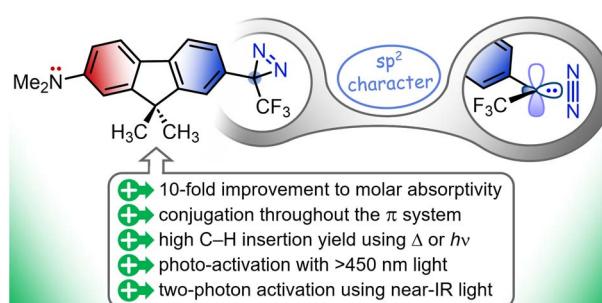
Yonggang Jiang, Hui Li, Haoqin Tang, Qingyue Zhang,  
Haitao Yang, Yu Pan, Chenggang Zou, Hongbin Zhang,\*  
Patrick J. Walsh\* and Xiaodong Yang\*



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**A diazirine's central carbon is sp<sup>2</sup>-hybridized, facilitating conjugation to dye molecules**

Lorenzo Michelini, Tanya Slaney, Seerat Virk,  
Estefanía Rafic, L. Charlie Qie, Klara Corejova,  
Mathieu L. Lepage, Stefania F. Musolino, Allen G. Oliver,  
Roberto Etchenique, W. David Hong,\* Gino A. DiLabio\*  
and Jeremy E. Wulff\*



## CORRECTION

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**Correction: An innovative chalcogenide transfer agent for improved aqueous quantum dot synthesis**

Guillaume Petit, Cedric Malherbe, Pauline Bianchi and Jean-Christophe M. Monbaliu\*

