

## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 16(2) 453–982 (2025)



**Cover**  
See Zheng Zhou and Marina A. Petrukhina, pp. 468–479.  
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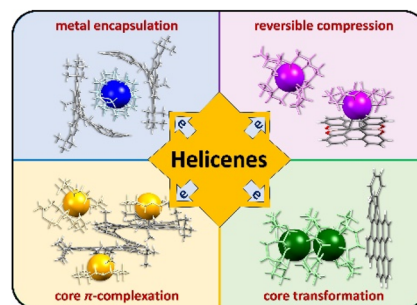
**Inside cover**  
See Renana Gershoni-Poranne *et al.*, pp. 575–583.  
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Image created by Dr. Vitalii Stetsovych.

## PERSPECTIVES

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

Zheng Zhou and Marina A. Petrukhina\*



480

### 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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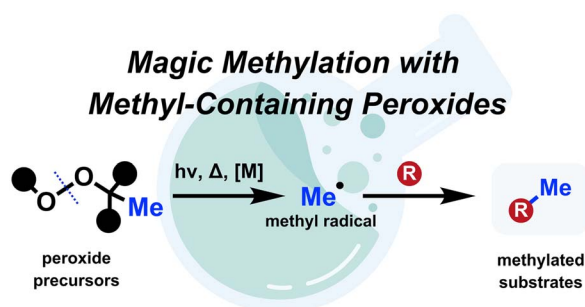
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## REVIEWS

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**Magic methylation with methyl-containing peroxides**

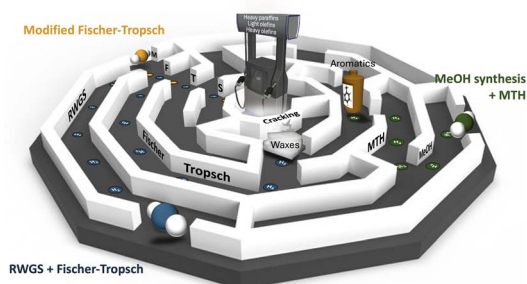
Daliah Farajat, Yuhua Zhang and Chao-Jun Li\*



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

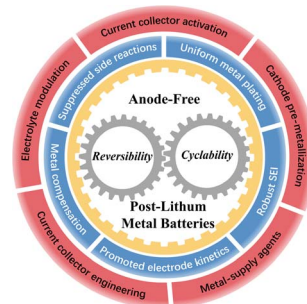
Enrique V. Ramos-Fernandez, Jose L. Santos, Dina K. Alsaadi, Anastasiya Bavykina, Jean Marcel R. Gallo and Jorge Gascon\*



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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\*

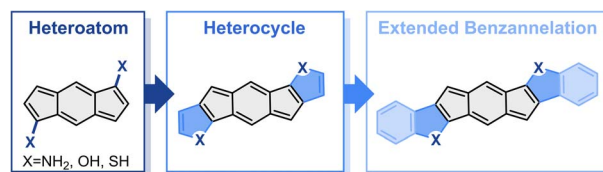


## EDGE ARTICLES

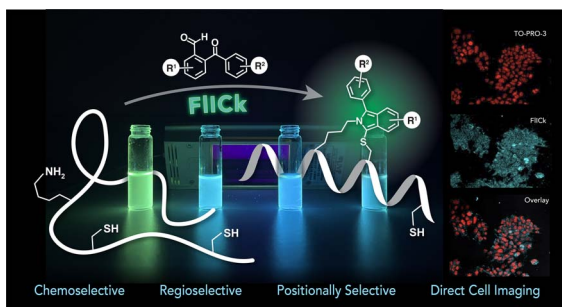
575

**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\*



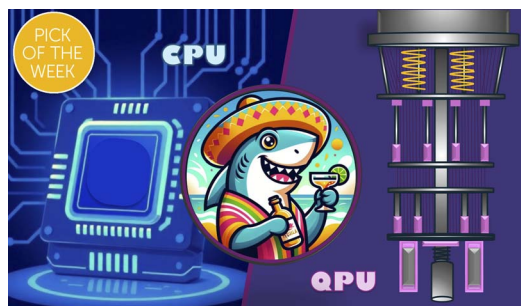
584



### 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\*

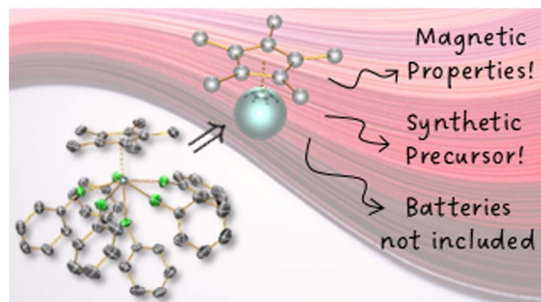
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### SHARC meets TEQUILA: mixed quantum-classical dynamics on a quantum computer using a hybrid quantum-classical algorithm

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

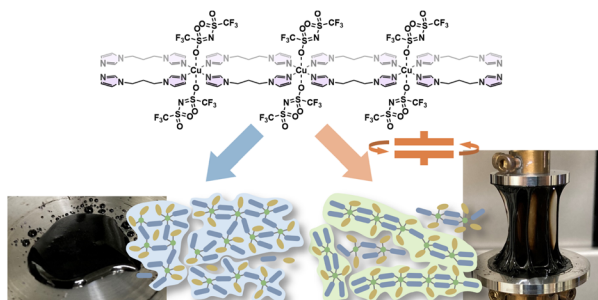
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### A fluorobenzene-bound dysprosium half-sandwich dication single-molecule magnet

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

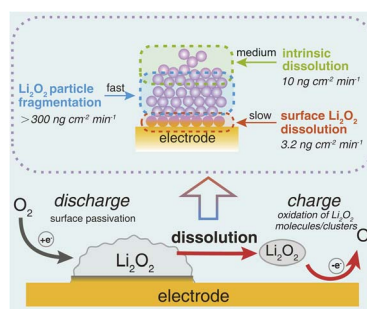
Taichi Nishiguchi, Yuki Ohara, Kentaro Kadota, Xin Zheng, Shin-ichiro Noro and Satoshi Horike\*



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

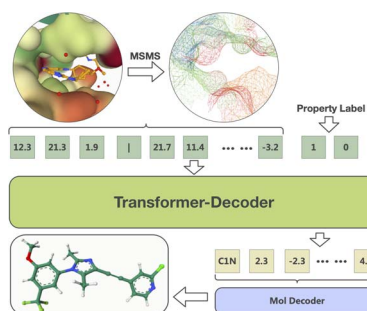
Lu He, Shuo Wang, Fengjiao Yu and Yuhui Chen\*



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

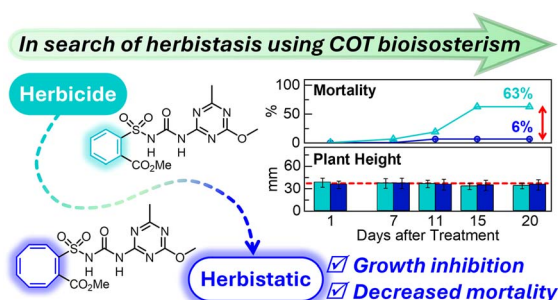
Jike Wang, Hao Luo, Rui Qin, Mingyang Wang, Xiaozhe Wan, Meijing Fang, Odin Zhang, Qiaolin Gou, Qun Su, Chao Shen, Ziyi You, Liwei Liu,\* Chang-Yu Hsieh,\* Tingjun Hou\* and Yu Kang\*



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

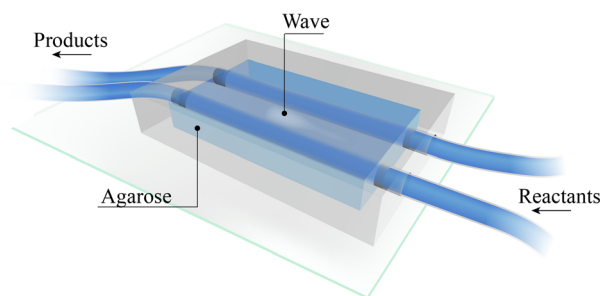
Hui Xing, Sarah K. M. McGregor, Bruna D. Batista, Cassidy Whitefield, Isobella S. J. Stone, Cody-Ellen Murray, Rebecca M. Hurst, Yizhou Liu, Sharon Chow, Tyler Fahrenhorst-Jones, Qi Zhao, Sevan D. Houston, Shu-Hong Hu, Thierry Lonhienne, Amanda Nouwens, Jed M. Burns, G. Paul Savage, Gimme H. Walter,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



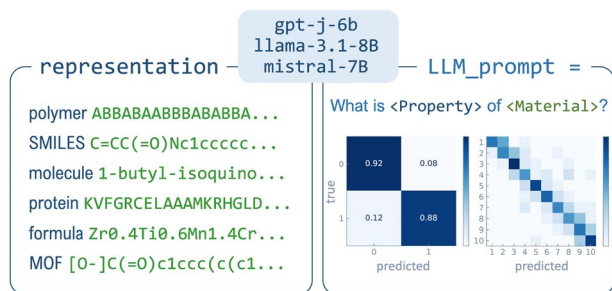
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## Chemical waves in reaction-diffusion networks of small organic molecules

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\*



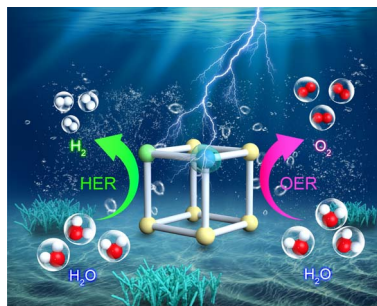
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## Assessment of fine-tuned large language models for real-world chemistry and material science applications

Joren Van Herck *et al.*

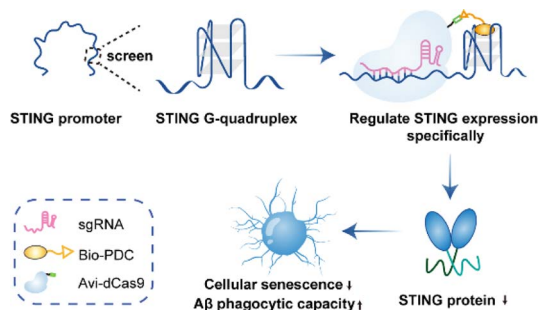
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## Rare-earth element doped NiFe-MOFs as efficient and robust bifunctional electrocatalysts for both alkaline freshwater and seawater splitting

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

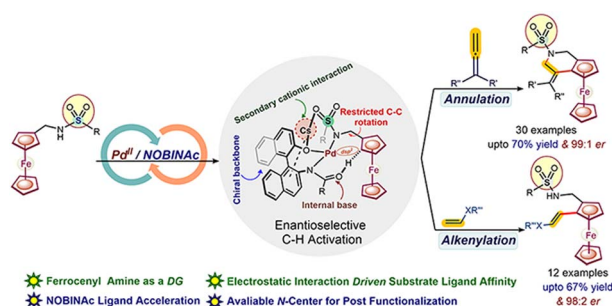
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## Regulation of STING G-quadruplex for rescuing cellular senescence and Aβ phagocytic capacity of microglia

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

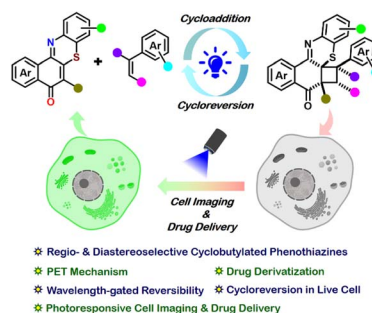
Devendra Parganiha, Raviraj Ananda Thorat, Ashwini Dilip Dhumale, Yagya Dutt Upadhyay, Raushan Kumar Jha, Saravanan Raju and Sangit Kumar\*



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

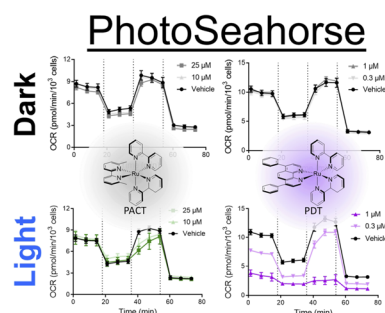
Sanhati Sharangi, Barsha Chakraborty, Raushan Kumar Jha, Swarnadeep Mandal, Apurba Lal Koner\* and Sangit Kumar\*



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### Photodynamic therapy photosensitizers and photoactivated chemotherapeutics exhibit distinct bioenergetic profiles to impact ATP metabolism

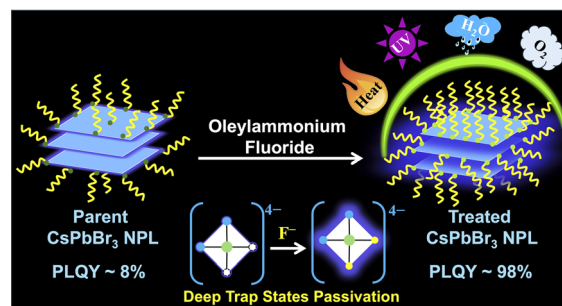
Richard J. Mitchell, Dmytro Havrylyuk, Austin C. Hachey, David K. Heidary\* and Edith C. Glazer\*



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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

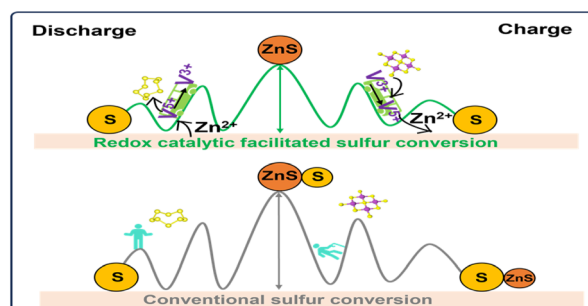
Arghya Sen, Abhijit Dutta, Abir Lal Bose and Pratik Sen\*



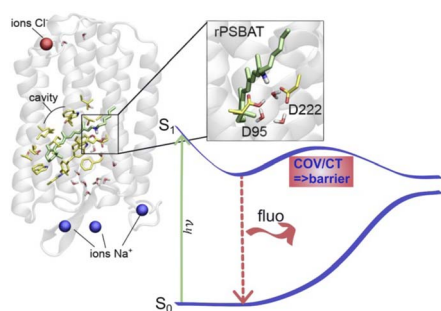
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### Reconstructing the phase of vanadium oxides enables redox-catalysis manipulated reversible sulfur conversion for stable Zn–S batteries

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



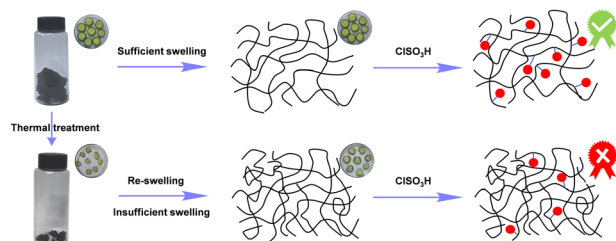
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### Archaelhodopsin 3 is an ideal template for the engineering of highly fluorescent optogenetic reporters

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

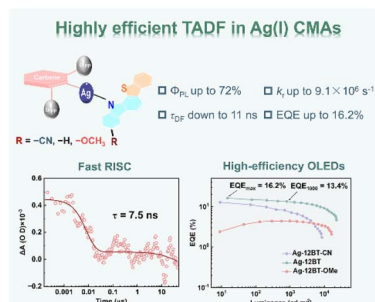
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### Efficient construction of high-quality sulfonated porous aromatic frameworks by optimizing the swelling state of porous structures

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

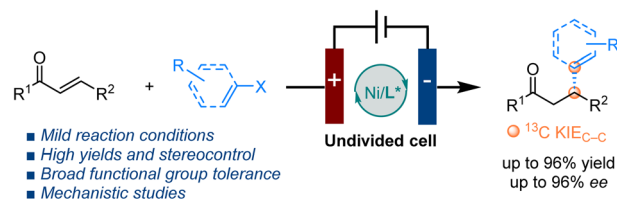
Yifan Yu, Min Ji, Yong Wang, Xuehui Yan, Lizhi Dai, Ningning Ma, Zhaoyu Zhou, Hang Xing and Ye Tian\*



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

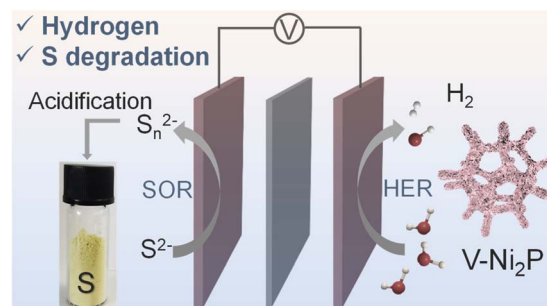
Siriphong Somprasong,\* Bin Wan and Syuzanna R. Harutyunyan\*



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### Vanadium-regulated nickel phosphide nanosheets for electrocatalytic sulfon upgrading and hydrogen production

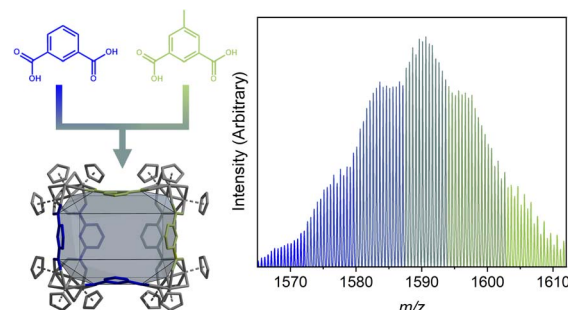
Rui-Qing Li,\* Xiaojun Wang, Shuixiang Xie, Songyun Guo, Zhe Cao, Zhenhao Yan, Wei Zhang\* and Xiaoyu Wan\*



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

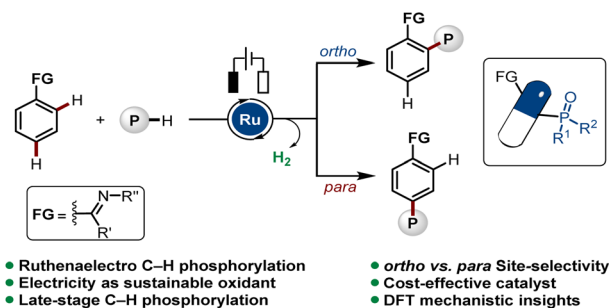
Merissa N. Morey, Christine M. Montone, Michael R. Dworzak, Glenn P. A. Yap and Eric D. Bloch\*



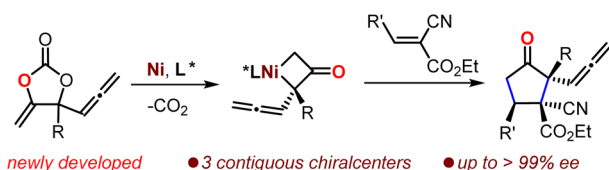
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### Ruthenaelectro-catalyzed C–H phosphorylation: *ortho* to *para* position-selectivity switch

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



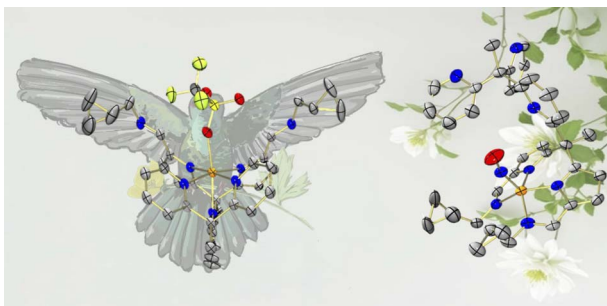
834



### 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\*

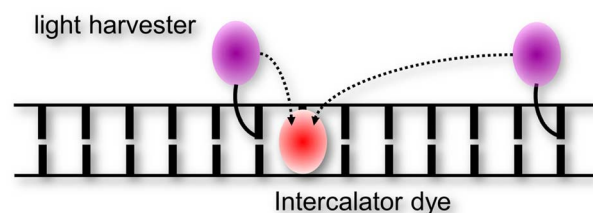
840



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

Jewelianna M. Moore and Alison R. Fout\*

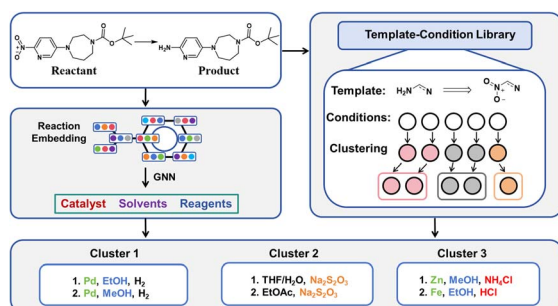
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### Light harvesting FIT DNA hybridization probes for brightness-enhanced RNA detection

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

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

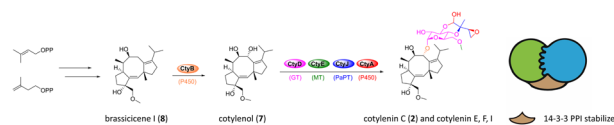
Zihan Wang, Kangjie Lin, Jianfeng Pei\* and Luhua Lai\*



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

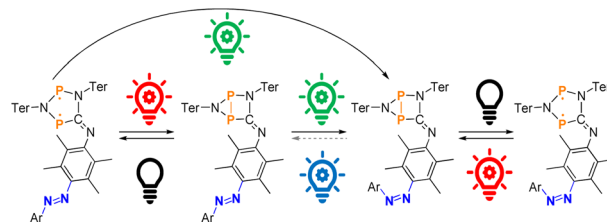
Zhenhua Guan, Nanyu Yao, Wenling Yuan, Fengli Li, Yang Xiao, Mewlude Rehmulla, Yuhua Xie, Chunmei Chen, Hucheng Zhu, Yuan Zhou, Qingyi Tong, Zheng Xiang\*, Ying Ye\* and Yonghui Zhang\*



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

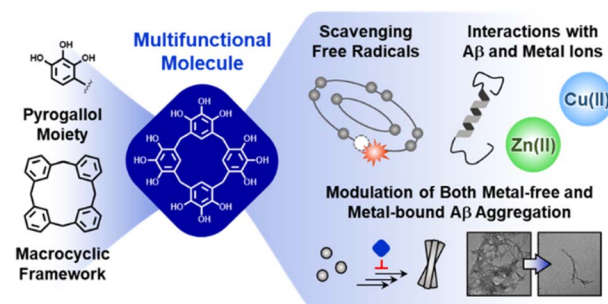
Yannic Pilopp, Henrik Beer, Jonas Bresien, Dirk Michalik, Alexander Villinger and Axel Schulz\*



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

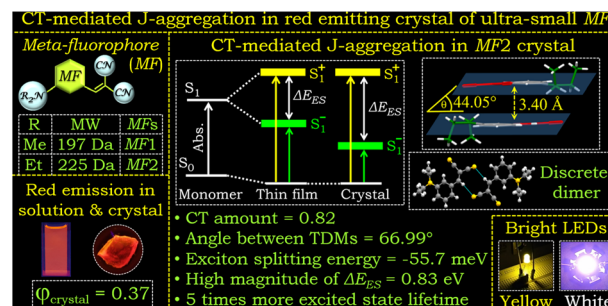
Jimin Kwak, Yelim Yi, Seongmin Park and Mi Hee Lim\*



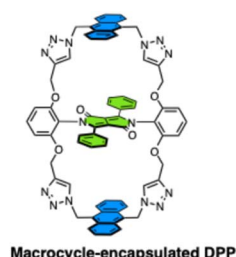
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## Charge-transfer mediated J-aggregation in red emitting ultra-small-single-benzenic meta-fluorophore crystals

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



910

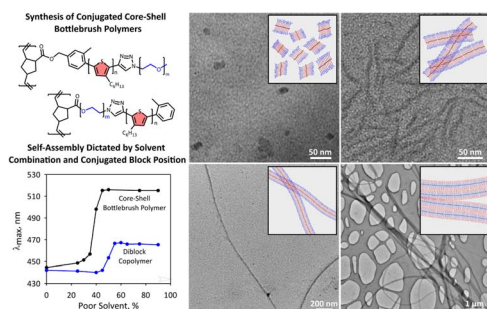


- ✓ Dual-state emission
- ✓ Intramolecular energy transfer
- ✓ Cu<sup>2+</sup> sensing
- ✓ Construction of self-threading polymer
- ✓ Mechanochromism

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

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

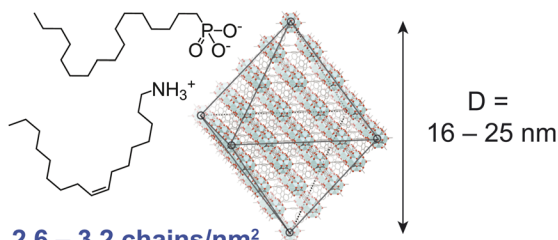
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### Conjugated core-shell bottlebrush polymers that exhibit crystallization-driven self-assembly

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

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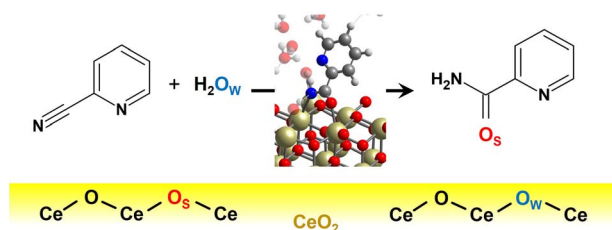


*Sterically Stabilized MOF Nanocrystal Colloids*

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

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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<sup>\*</sup> and Akira Nakayama<sup>\*</sup>

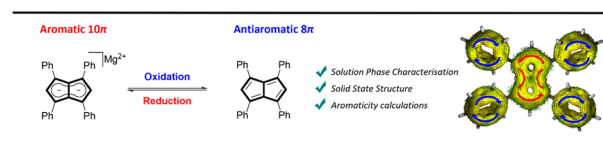


## EDGE ARTICLES

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

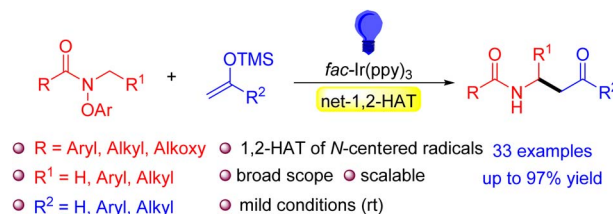
Hugh J. Sanderson, Andreas Helbig, Gabriele Kociok-Köhn, Holger Helten\* and Ulrich Hintermair\*



962

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

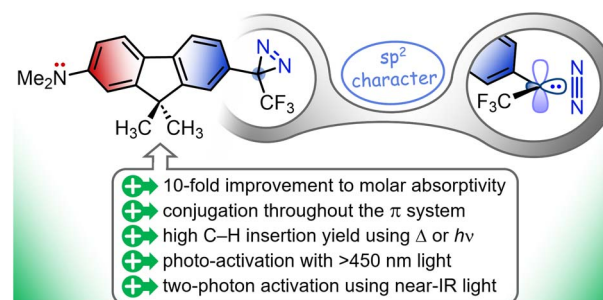
Yonggang Jiang, Hui Li, Haoqin Tang, Qingyue Zhang, Haitao Yang, Yu Pan, Chenggang Zou, Hongbin Zhang,\* Patrick J. Walsh\* and Xiaodong Yang\*



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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

980

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

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

