

## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(12) 4189–4604 (2024)



**Cover**  
See Chengchao Xu, Huan Tang, Jigang Wang *et al.*, pp. 4313–4321. Image reproduced by permission of Jigang Wang from *Chem. Sci.*, 2024, 15, 4313.



**Inside cover**  
See Kirill Yu. Monakhov *et al.*, pp. 4202–4221. Image reproduced by permission of Kirill Yu. Monakhov from *Chem. Sci.*, 2024, 15, 4202.

## PERSPECTIVES

4202

### Bioorthogonal chemistry of polyoxometalates – challenges and prospects

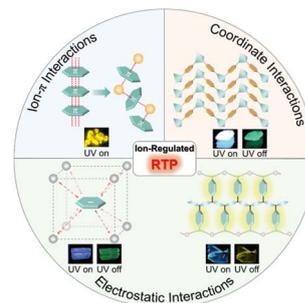
Stanislav K. Petrovskii, Elena V. Grachova and Kirill Yu. Monakhov\*



4222

### Recent progress in ion-regulated organic room-temperature phosphorescence

Wenbo Dai, Yitian Jiang, Yunxiang Lei, Xiaobo Huang, Peng Sun, Jianbing Shi, Bin Tong, Dongpeng Yan,\* Zhengxu Cai\* and Yuping Dong



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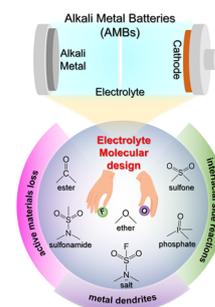
Fundamental questions  
Elemental answers

## REVIEWS

4238

## Recent advances in electrolyte molecular design for alkali metal batteries

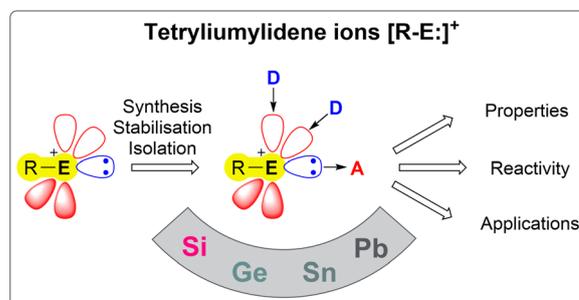
Digen Ruan, Zhuangzhuang Cui, Jiajia Fan, Dazhuang Wang, Yiyang Wu\* and Xiaodi Ren\*



4275

## Tetryliumylidene ions in synthesis and catalysis

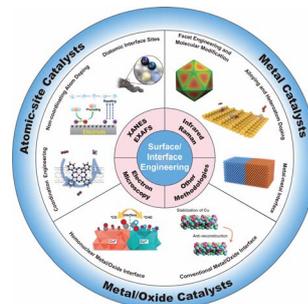
Sebastian Stigler, Shiori Fujimori, Arseni Kostenko and Shigeyoshi Inoue\*



4292

Customizing catalyst surface/interface structures for electrochemical CO<sub>2</sub> reduction

Xin Tan, Haojie Zhu, Chang He, Zewen Zhuang, Kaian Sun, Chao Zhang\* and Chen Chen\*

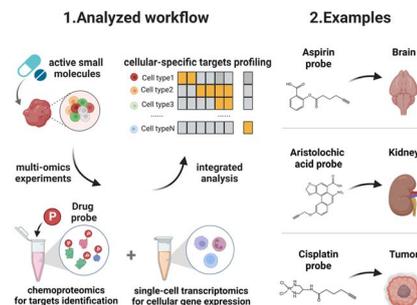


## EDGE ARTICLES

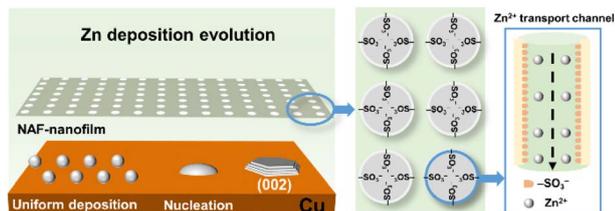
4313

STEP: profiling cellular-specific targets and pathways of bioactive small molecules in tissues *via* integrating single-cell transcriptomics and chemoproteomics

Jiayun Chen, Zheng Chu, Qian Zhang, Chen Wang, Piao Luo, Ying Zhang, Fei Xia, Liwei Gu, Yin Kwan Wong, Qiaoli Shi, Chengchao Xu,\* Huan Tang\* and Jigang Wang\*



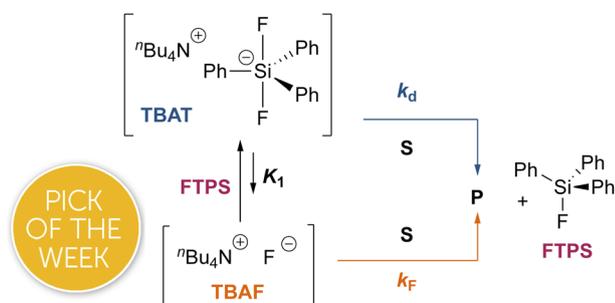
4322



### *In situ* Nafion-nanofilm oriented (002) Zn electrodeposition for long-term zinc-ion batteries

Da Zhang, Ziyang Song, Ling Miao, Yaokang Lv, Lihua Gan and Mingxian Liu\*

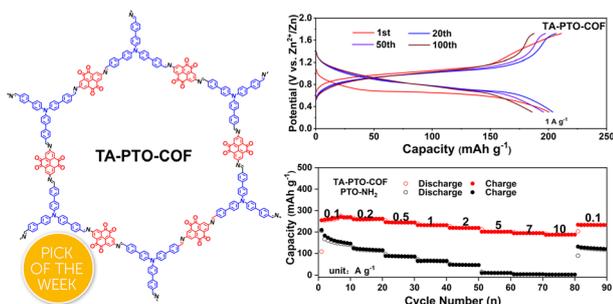
4331



### Speciation and kinetics of fluoride transfer from tetra-*n*-butylammonium difluorotriphenylsilicate ('TBAT')

Maciej M. Kucharski, Allan J. B. Watson and Guy C. Lloyd-Jones\*

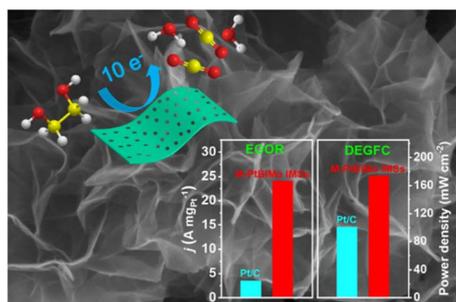
4341



### A covalent organic framework as a dual-active-center cathode for a high-performance aqueous zinc-ion battery

Hongbao Li, Mengge Cao, Zhenli Fu, Quanwei Ma, Longhai Zhang, Rui Wang, Fei Liang, Tengfei Zhou and Chaofeng Zhang\*

4349



### Mesoporous Mo-doped PtBi intermetallic metallene superstructures to enable the complete electrooxidation of ethylene glycol

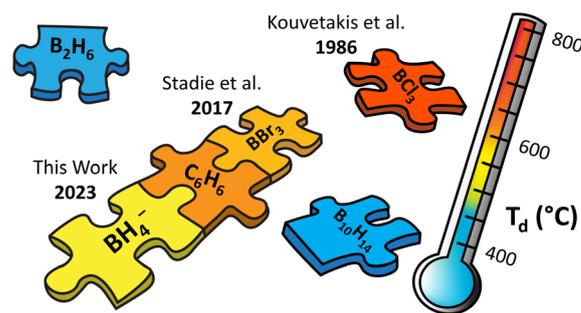
Xiaotong Yang, Qiang Yuan,\* Tian Sheng\* and Xun Wang\*



4358

**Halide-free synthesis of metastable graphitic BC<sub>3</sub>**

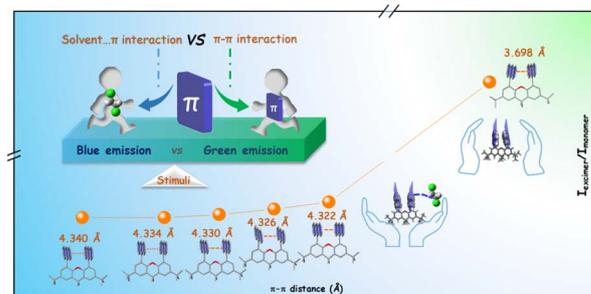
Devin McGlamery, Charles McDaniel, Dylan M. Ladd, Yang Ha, Martin A. Mosquera, Michael T. Mock and Nicholas P. Stadie\*



4364

**Controllable  $\pi$ - $\pi$  coupling of intramolecular dimer models in aggregated states**

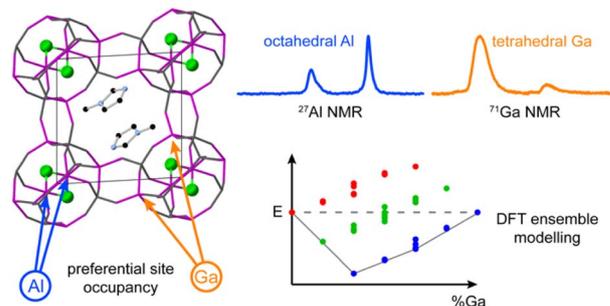
Qiuyan Liao, Aisen Li, Arui Huang, Jiaqiang Wang, Kai Chang, Hehua Li, Pengfei Yao, Cheng Zhong, Peidong Xie, Jinfeng Wang, Zhen Li\* and Qianqian Li\*



4374

**Site-directed cation ordering in chabazite-type Al<sub>x</sub>Ga<sub>1-x</sub>PO<sub>4</sub>-34 frameworks revealed by NMR crystallography**

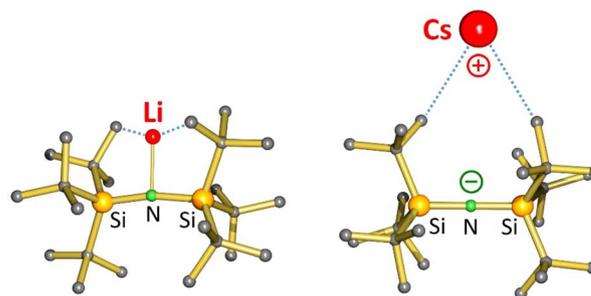
Daniel M. Dawson,\* Jasmine A. Clayton, Thomas H. D. Marshall, Nathalie Guillou, Richard I. Walton\* and Sharon E. Ashbrook\*



4386

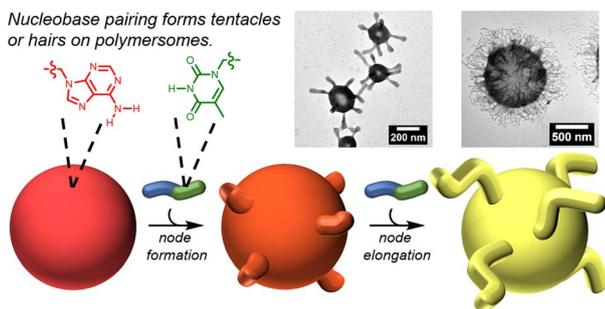
**s-Block metal complexes of superbuly (<sup>t</sup>Bu<sub>3</sub>Si)<sub>2</sub>N<sup>-</sup>: a new weakly coordinating anion?**

Christian Knüpfel, Lukas Klerner, Jonathan Mai, Jens Langer and Sjoerd Harder\*



4396

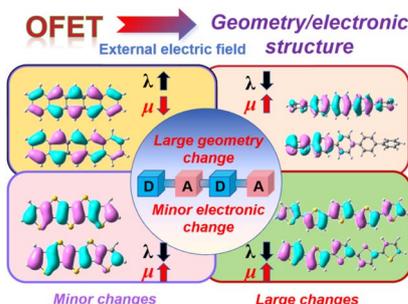
Nucleobase pairing forms tentacles or hairs on polymersomes.



### Controlled node growth on the surface of polymersomes

Marjolaine Thomas, Spyridon Varlas, Thomas R. Wilks, Stephen D. P. Fielden\* and Rachel K. O'Reilly\*

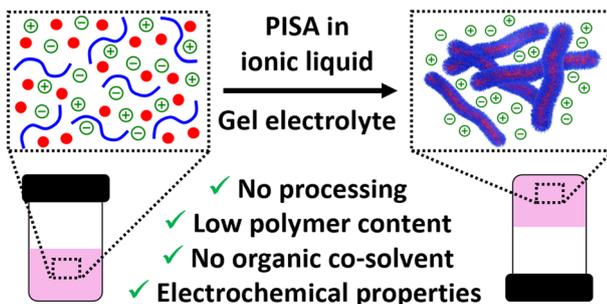
4403



### In-depth theoretical analysis of the influence of an external electric field on charge transport parameters

Gui-Ya Qin, Xiao-Qi Sun, Rui Wang, Jing-Fu Guo, Jian-Xun Fan, Hui Li, Lu-Yi Zou and Ai-Min Ren\*

4416



### Block copolymer synthesis in ionic liquid via polymerisation-induced self-assembly: a convenient route to gel electrolytes

Georgia L. Maitland, Mingyu Liu, Thomas J. Neal, James Hammerton, Yisong Han, Stephen D. Worrall, Paul D. Topham and Matthew J. Derry\*

4427



### Wavelength-dependent rearrangements of an $\alpha$ -dione chromophore: a chemical pearl in a bis(hypersilyl) oyster

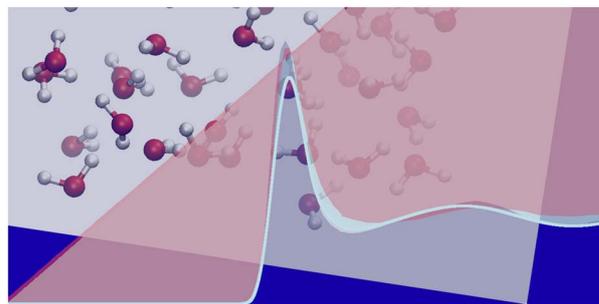
Gabriel Glotz, Manfred Drusgala, Florian Hamm, Roland C. Fischer, Nađa Došlić, Anne-Marie Kelterer, Georg Gescheidt\* and Michael Haas\*



4434

### Structure and dynamics of liquid water from *ab initio* simulations: adding Minnesota density functionals to Jacob's ladder

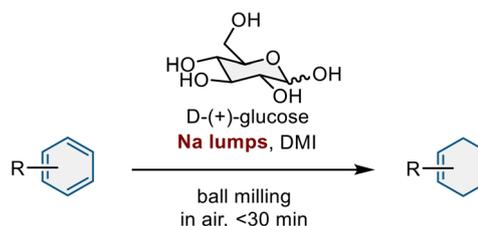
Justin Villard, Martin P. Bircher and Ursula Rothlisberger\*



4452

### Mechanochemistry enabling highly efficient Birch reduction using sodium lumps and D-(+)-glucose

Keisuke Kondo, Koji Kubota\* and Hajime Ito\*

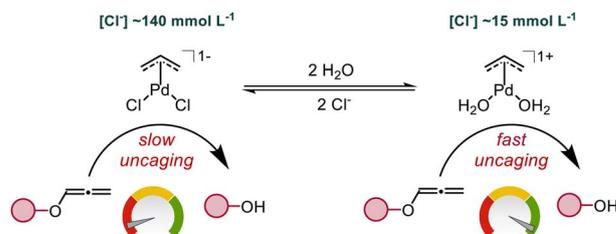


- cheap and shelf-stable sodium source
- fast, air-tolerant and bulk solvent-free

4458

### Interplay of chloride levels and palladium(II)-catalyzed *O*-deallylation bioorthogonal uncaging reactions

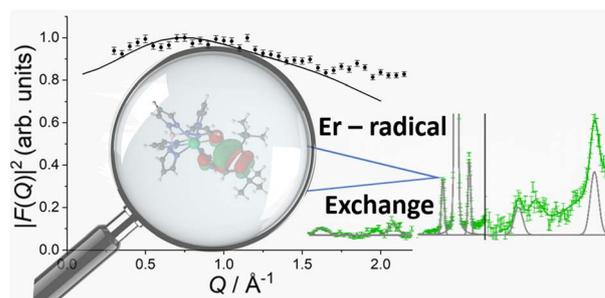
Gean M. Dal Forno, Eloah Latocheski, Claudio D. Navo, Brunno L. Albuquerque, Albert L. St John, Frédéric Avenier, Gonzalo Jiménez-Osés and Josiel B. Domingos\*



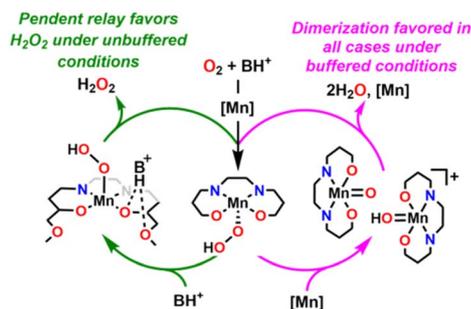
4466

### *Ab initio*-based determination of lanthanoid–radical exchange as visualised by inelastic neutron scattering

Maja A. Dunstan, Marcus J. Giansiracusa, Simone Calvello, Lorenzo Sorace, Anwen M. Krause-Heuer, Alessandro Soncini,\* Richard A. Mole\* and Colette Boskovic\*



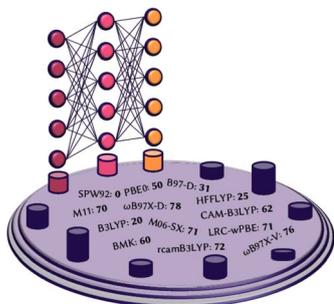
4478



### Controlling product selectivity during dioxygen reduction with Mn complexes using pendent proton donor relays and added base

Emma N. Cook, Ian M. Courter, Diane A. Dickie and Charles W. Machan\*

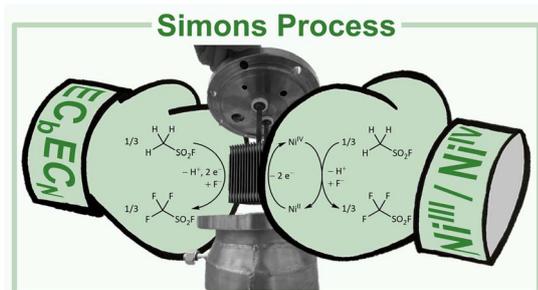
4489



### DELFI: a computer oracle for recommending density functionals for excited states calculations

Davide Avagliano,\* Marta Skreta, Sebastian Arellano-Rubach and Alán Aspuru-Guzik\*

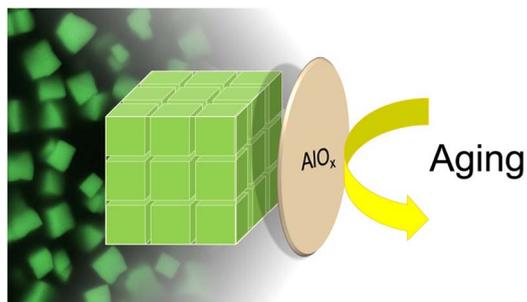
4504



### Unravelling highly oxidized nickel centers in the anodic black film formed during the Simons process by *in situ* X-ray absorption near edge structure spectroscopy

Gene Senges, Ana Guilherme Buzanich, Tilen Lindič, Tyler A. Gully, Marlon Winter, Martin Radtke, Bettina Röder, Simon Steinhauer, Beate Paulus, Franziska Emmerling and Sebastian Riedel\*

4510



### Long live(d) CsPbBr<sub>3</sub> superlattices: colloidal atomic layer deposition for structural stability

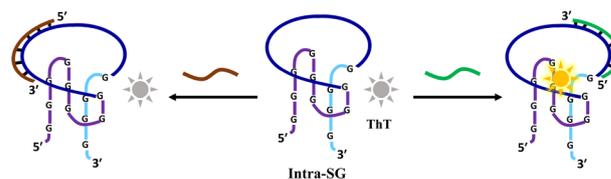
Victoria Lapointe, Philippe B. Green, Alexander N. Chen, Raffaella Buonsanti and Marek B. Majewski\*



4519

### Topological effect of an intramolecular split G-quadruplex on thioflavin T binding and fluorescence light-up

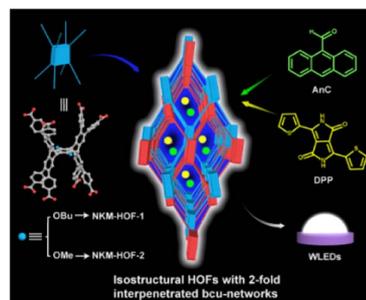
Mengmeng Lv, Jiangtao Ren\* and Erkang Wang\*



4529

### Reticular synthesis of 8-connected carboxyl hydrogen-bonded organic frameworks for white-light-emission

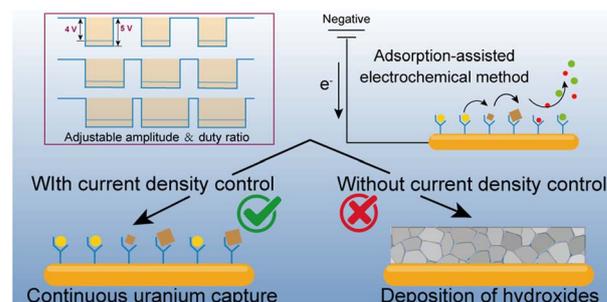
Xiao-Juan Xi, Yang Li, Feifan Lang, Jiandong Pang\* and Xian-He Bu\*



4538

### A marine bacteria-inspired electrochemical regulation for continuous uranium extraction from seawater and salt lake brine

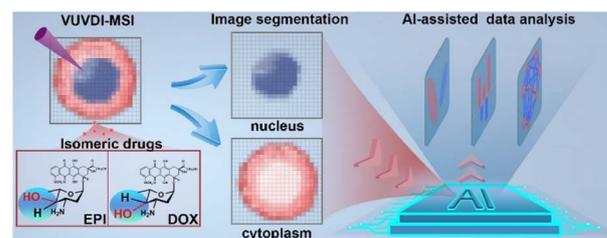
Linsen Yang, Yongchao Qian, Zehua Zhang, Tingyang Li, Xiangbin Lin, Lin Fu, Shengyang Zhou, Xiang-Yu Kong, Lei Jiang and Liping Wen\*



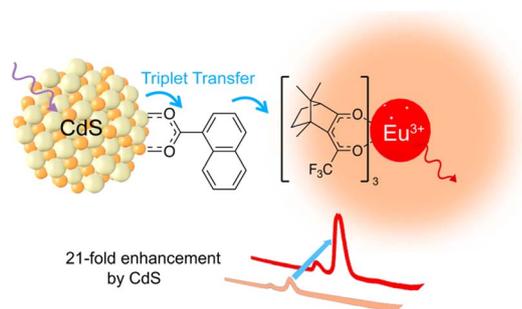
4547

### AI-assisted mass spectrometry imaging with *in situ* image segmentation for subcellular metabolomics analysis

Cong-Lin Zhao, Han-Zhang Mou, Jian-Bin Pan, Lei Xing,\* Yuxiang Mo, Bin Kang,\* Hong-Yuan Chen and Jing-Juan Xu\*



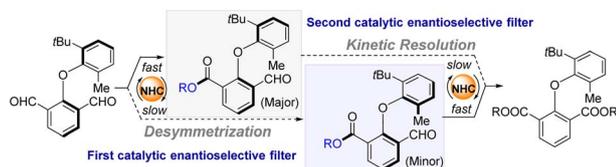
4556



### Triplet energy transfer from quantum dots increases Ln(III) photoluminescence, enabling excitation at visible wavelengths

Tingting Huang, Sheng He, Anji Ni, Tianquan Lian\* and Ming Lee Tang\*

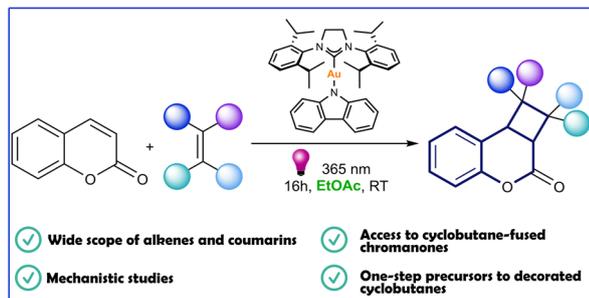
4564



### Synthesis of axially chiral diaryl ethers via NHC-catalyzed atroposelective esterification

Yingtao Wu, Xin Guan, Huaqiu Zhao, Mingrui Li, Tianlong Liang, Jiaqiong Sun, Guangfan Zheng\* and Qian Zhang\*

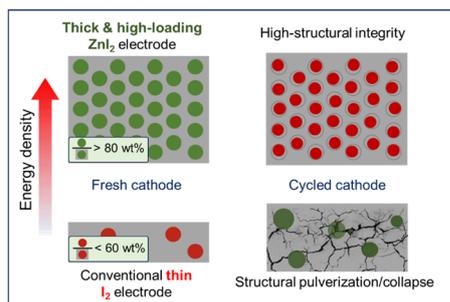
4571



### Synthesis of cyclobutane-fused chromanones via gold-mediated photocatalysis

Vladislav A. Voloshkin, Marco Villa, Ekaterina A. Martynova, Marek Beliš, Kristof Van Hecke, Paola Ceroni\* and Steven P. Nolan\*

4581



### Unleashing the high energy potential of zinc–iodide batteries: high-loaded thick electrodes designed with zinc iodide as the cathode

Jingkang Ma, Alireza Azizi, Erhuan Zhang, Hong Zhang,\* Anqiang Pan\* and Ke Lu\*



4590

## From $\pi$ -conjugated macrocycles to heterocycloarenes based on benzo[2,1-*b*:3,4-*b'*]dithiophene (BDTh): size- and geometry-dependent host-guest properties

Dongyue An, Rong Zhang, Jiangyu Zhu, Teng Wang, Yan Zhao, Xuefeng Lu\* and Yunqi Liu

