

# 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 15(7) 2269–2670 (2024)



**Cover**  
See Takahiro Muraoka, Masaki Okumura, Tomohide Saio, pp. 2282–2299. Image reproduced by permission of Takahiro Muraoka from *Chem. Sci.*, 2024, 15, 2282.



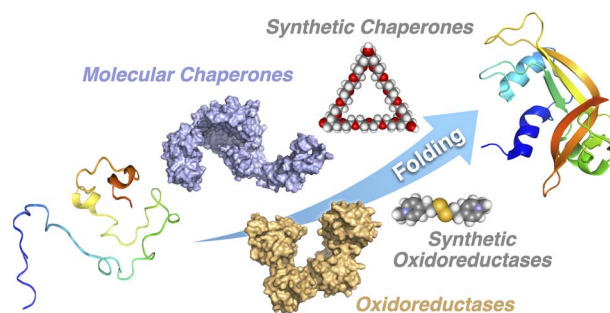
**Inside cover**  
See Antonio Leyva-Pérez, Carlos Martí-Gastaldo *et al.*, pp. 2351–2358. Image reproduced by permission of Carmen Fernández-Conde from *Chem. Sci.*, 2024, 15, 2351.

## PERSPECTIVES

2282

### Enzymatic and synthetic regulation of polypeptide folding

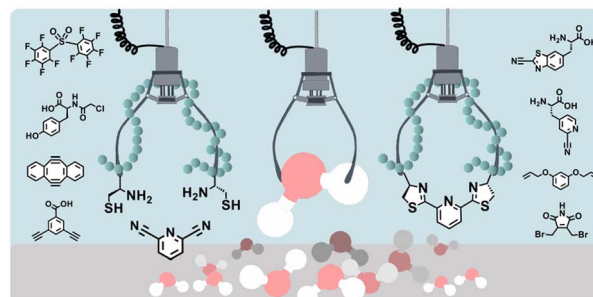
Takahiro Muraoka,\* Masaki Okumura\* and Tomohide Saio\*



2300

### Biocompatible strategies for peptide macrocyclisation

Junming He, Pritha Ghosh and Christoph Nitsche\*



# RSC Applied Polymers

GOLD  
OPEN  
ACCESS

The application of polymers,  
both natural and synthetic

Interdisciplinary and open access

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

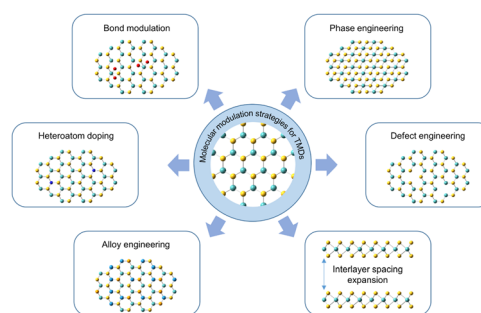
Fundamental questions  
Elemental answers

## REVIEW

2323

## Molecular modulation strategies for two-dimensional transition metal dichalcogenide-based high-performance electrodes for metal-ion batteries

Mingyuan Gu, Apparao M. Rao, Jiang Zhou and Bingan Lu\*

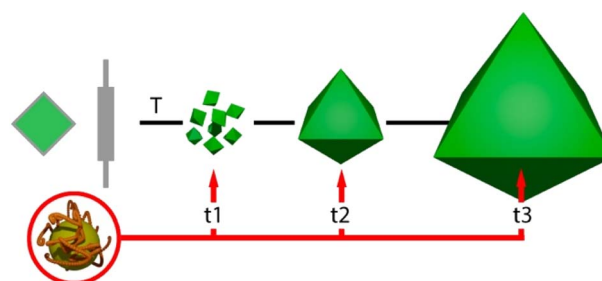


## EDGE ARTICLES

2351

## Time-resolved control of nanoparticle integration in titanium-organic frameworks for enhanced catalytic performance

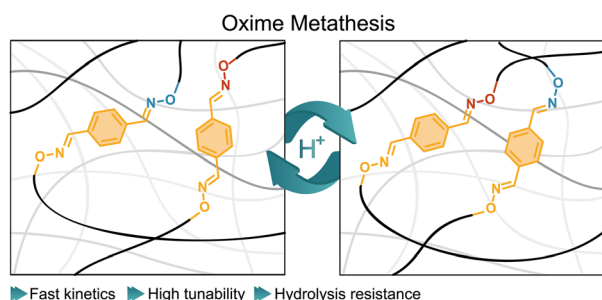
Carmen Fernández-Conde, Yongkun Zheng, Marta Mon, Antonio Ribera, Antonio Leyva-Pérez\* and Carlos Martí-Gastaldo\*



2359

## Oxime metathesis: tuneable and versatile chemistry for dynamic networks

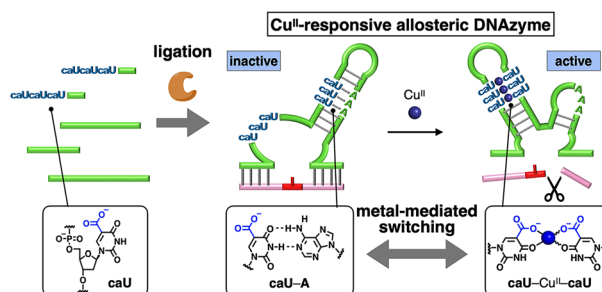
Luca Pettazoni, Marta Ximenis, Francesca Leonelli, Giulia Vozzolo, Enrico Bodo, Fermin Elizalde and Haritz Sardon\*



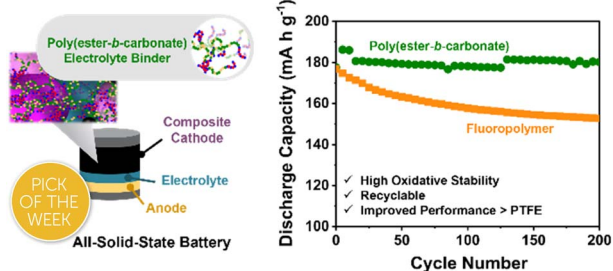
2365

## Ligase-mediated synthesis of Cu<sup>II</sup>-responsive allosteric DNAzyme with bifacial 5-carboxyuracil nucleobases

Yusuke Takezawa,\* Hanci Zhang, Keita Mori, Lingyun Hu and Mitsuhiro Shionoya\*



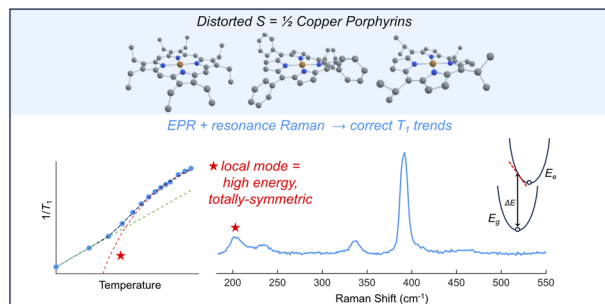
2371



### Alternatives to fluorinated binders: recyclable copolyester/carbonate electrolytes for high-capacity solid composite cathodes

Holly Yeo, Georgina L. Gregory,\* Hui Gao, Kanyapat Yiamsawat, Gregory J. Rees, Thomas McGuire, Mauro Pasta,\* Peter G. Bruce\* and Charlotte K. Williams\*

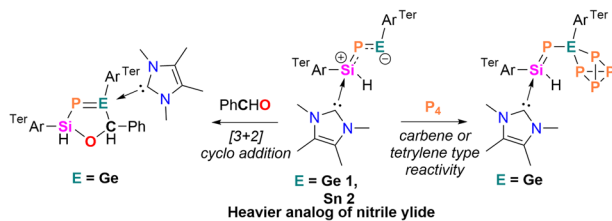
2380



### Determining the key vibrations for spin relaxation in ruffled Cu(II) porphyrins via resonance Raman spectroscopy

Nathanael P. Kazmierczak, Nathan E. Lopez, Kaitlin M. Luedecke and Ryan G. Hadt\*

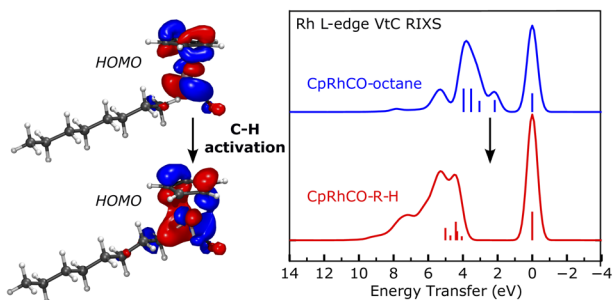
2391



### Synthesis and reactivity of N-heterocyclic carbene (NHC)-supported heavier nitrile ylides

Debotra Sarkar, Sayan Dutta, Franziska Hanusch, Debasis Koley\* and Shigeyoshi Inoue\*

2398



### Accessing metal-specific orbital interactions in C–H activation with resonant inelastic X-ray scattering

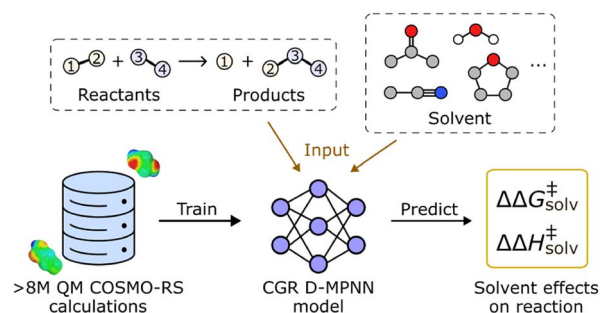
Ambar Banerjee,\* Raphael M. Jay,\* Torsten Leitner, Ru-Pan Wang, Jessica Harich, Robert Stefanuik, Michael R. Coates, Emma V. Beale, Victoria Kabanova, Abdullah Kahraman, Anna Wach, Dmitry Ozerov, Christopher Arrell, Christopher Milne, Philip J. M. Johnson, Claudio Cirelli, Camila Bacellar, Nils Huse, Michael Odelius\* and Philippe Wernet\*



2410

## Machine learning from quantum chemistry to predict experimental solvent effects on reaction rates

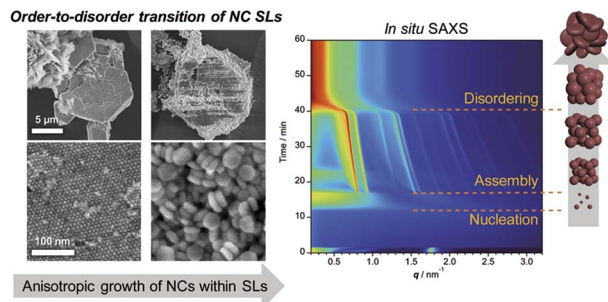
Yunsie Chung and William H. Green\*



2425

## Pseudomorphic amorphization of three-dimensional superlattices through morphological transformation of nanocrystal building blocks

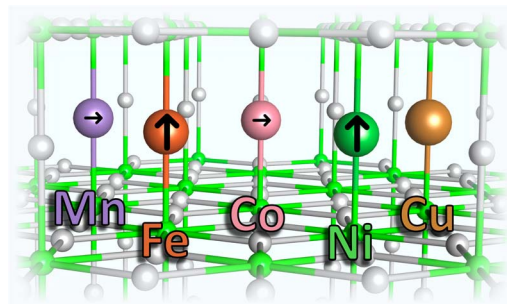
Masaki Saruyama,\* Ryo Takahata, Ryota Sato, Kenshi Matsumoto, Lingkai Zhu, Yohei Nakanishi, Motoki Shibata, Tomotaka Nakatani, So Fujinami, Tsukasa Miyazaki, Mikihiro Takenaka and Toshiharu Teranishi\*



2433

## Quantifying the influence of 3d–4s mixing on linearly coordinated metal-ions by $L_{2,3}$ -edge XAS and XMCD

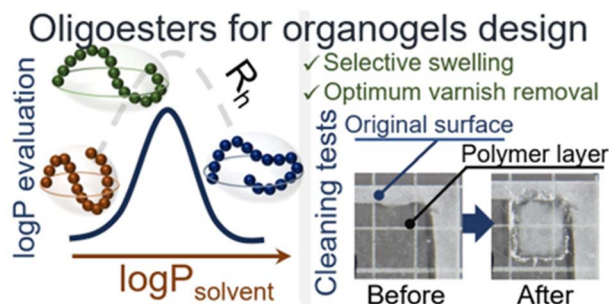
Myron S. Huzan, Timothy G. Burrow, Manuel Fix, Franziska A. Breitner, Sut Kei Chong, Peter Bencok, Matteo Aramini, Anton Jesche and Michael L. Baker\*



2443

## New sustainable polymers and oligomers for Cultural Heritage conservation

Damiano Bandelli, Rosangela Mastrangelo, Giovanna Poggi, David Chelazzi\* and Piero Baglioni\*



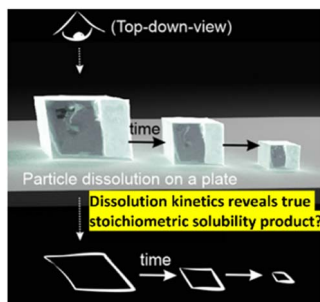
2456



### Modular, multi-robot integration of laboratories: an autonomous workflow for solid-state chemistry

Amy. M. Lunt, Hatem Fakhruddin, Gabriella Pizzuto, Louis Longley, Alexander White, Nicola Rankin, Rob Clowes, Ben Alston, Lucia Gigli, Graeme M. Day, Andrew I. Cooper\* and Samantha Y. Chong\*

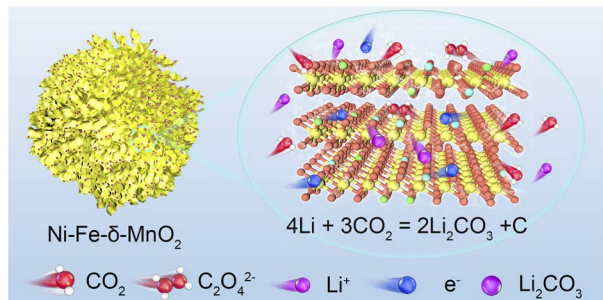
2464



### The solubility product controls the rate of calcite dissolution in pure water and seawater

Minjun Yang, Ling Tan, Christopher Batchelor-McAuley and Richard G. Compton\*

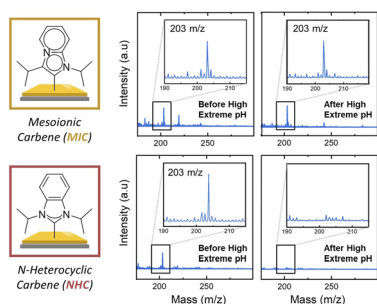
2473



### Facile fabrication of Ni, Fe-doped $\delta$ -MnO<sub>2</sub> derived from Prussian blue analogues as an efficient catalyst for stable Li-CO<sub>2</sub> batteries

Xiaoyang Chen, Jian Chen, Yun Qiao,\* Yun Gao, Siwei Fan, Yijie Liu, Li Li, Yang Liu\* and Shulei Chou\*

2480



### Mesoionic carbene-based self-assembled monolayers on gold

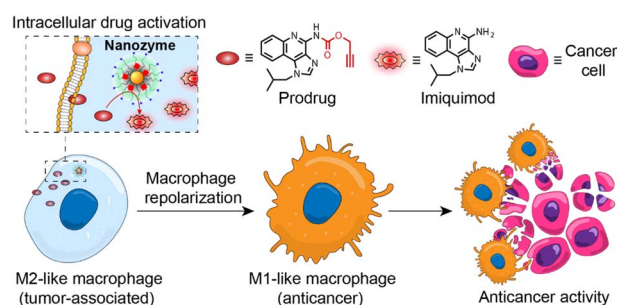
Dianne S. Lee, Ishwar Singh, Alex J. Veinot, Mark D. Aloisio, Justin T. Lomax, Paul J. Ragogna and Cathleen M. Crudden\*



2486

### Polarization of macrophages to an anti-cancer phenotype through *in situ* uncaging of a TLR 7/8 agonist using bioorthogonal nanozymes

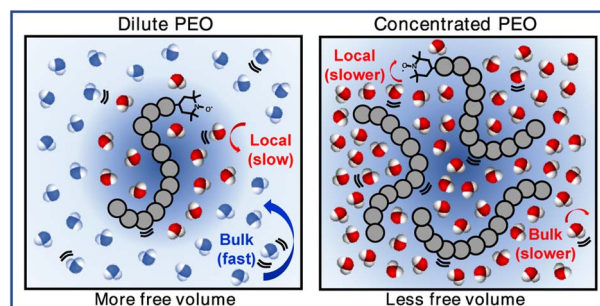
Xianzhi Zhang, Yuanchang Liu, Mingdi Jiang, Javier A. Mas-Rosario, Stefano Fedeli, Roberto Cao-Milan, Liang Liu, Kyle J. Winters, Cristina-Maria Hirschbiegel, Ahmed Nabawy, Rui Huang, Michelle E. Farkas and Vincent M. Rotello\*



2495

### Nanoscale water-polymer interactions tune macroscopic diffusivity of water in aqueous poly(ethylene oxide) solutions

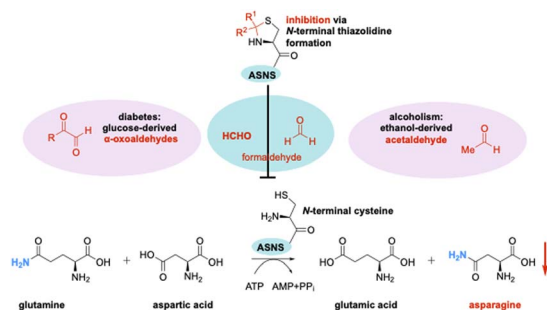
Joshua D. Moon, Thomas R. Webber, Dennis Robinson Brown, Peter M. Richardson, Thomas M. Casey, Rachel A. Segalman, M. Scott Shell and Songji Han\*



2509

### Aldehyde-mediated inhibition of asparagine biosynthesis has implications for diabetes and alcoholism

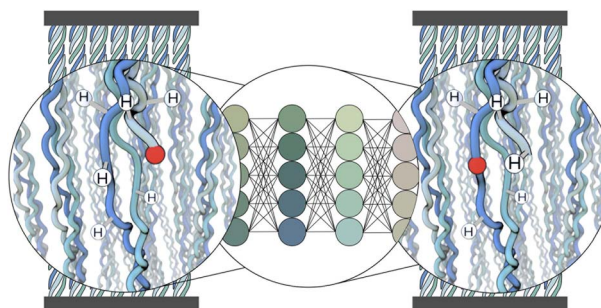
Tobias John, Nadia Saffoon, John Walsby-Tickle, Svenja S. Hester, Felix A. Dingler, Christopher L. Millington, James S. O. McCullagh, Ketan J. Patel, Richard J. Hopkinson\* and Christopher J. Schofield\*



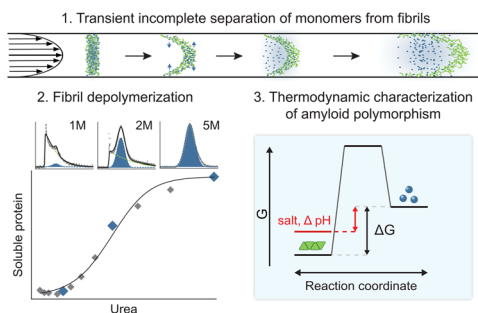
2518

### Substituting density functional theory in reaction barrier calculations for hydrogen atom transfer in proteins

Kai Riedmiller, Patrick Reiser, Elizaveta Bobkova, Kiril Maltsev, Ganna Gryn'ova, Pascal Friederich\* and Frauke Gräter\*



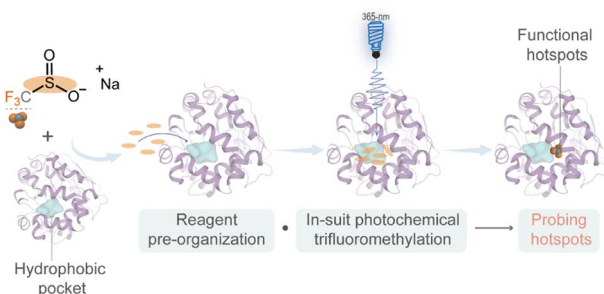
2528



### Thermodynamic characterization of amyloid polymorphism by microfluidic transient incomplete separation

Azad Farzadfard, Antonin Kunka, Thomas Oliver Mason, Jacob Aunstrup Larsen, Rasmus Krogh Norrild, Elisa Torrescasana Dominguez, Soumik Ray and Alexander K. Buell\*

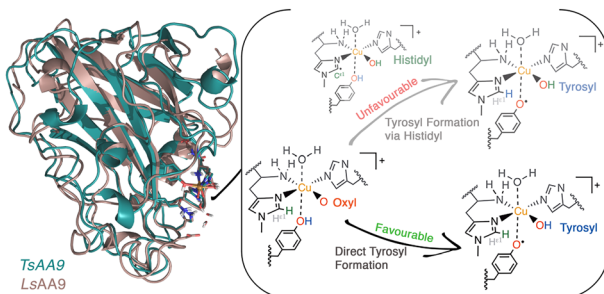
2545



### Probing the functional hotspots inside protein hydrophobic pockets by *in situ* photochemical trifluoromethylation and mass spectrometry

Can Lai, Zhiyao Tang, Zheyi Liu, Pan Luo, Wenxiang Zhang, Tingting Zhang, Wenhao Zhang, Zhe Dong,\* Xinyuan Liu, Xueming Yang and Fangjun Wang\*

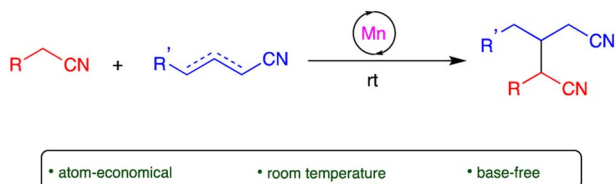
2558



### Understanding the initial events of the oxidative damage and protection mechanisms of the AA9 lytic polysaccharide monoxygenase family

Marlisa M. Hagemann, Erna K. Wieduwilt and Erik D. Hedegård\*

2571



### Manganese-catalyzed base-free addition of saturated nitriles to unsaturated nitriles by template catalysis

Subramanian Thiyagarajan, Yael Diskin-Posner, Michael Montag and David Milstein\*

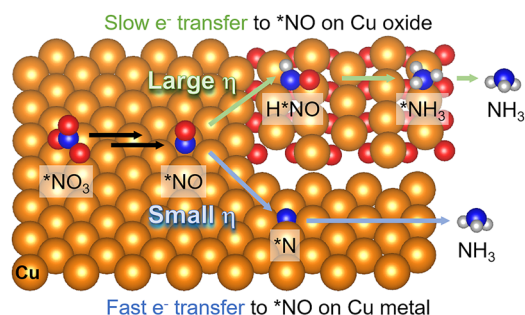




2578

### Identifying the active sites and intermediates on copper surfaces for electrochemical nitrate reduction to ammonia

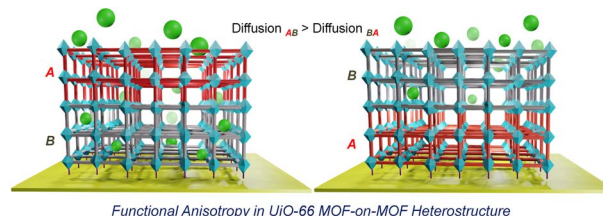
Yohan Kim, Jinyoung Ko, Minyoung Shim, Jiwon Park, Hyun-Hang Shin, Zee Hwan Kim, Yousung Jung\* and Hye Ryung Byon\*



2586

### Leveraging metal node-linker self-assembly to access functional anisotropy of zirconium-based MOF-on-MOF epitaxial heterostructure thin films

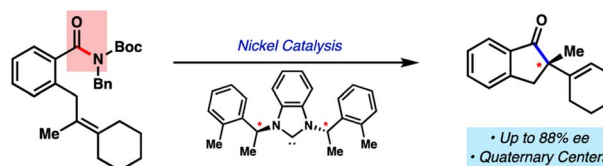
Suvendu Panda, Susmita Kundu, Pratibha Malik and Ritesh Halder\*



2593

### Enantioselective nickel-catalyzed Mizoroki–Heck cyclizations of amide electrophiles

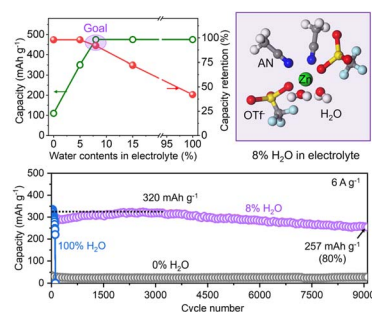
Ana S. Bulger, Daniel J. Nasrallah, Arismel Tena Meza and Neil K. Garg\*



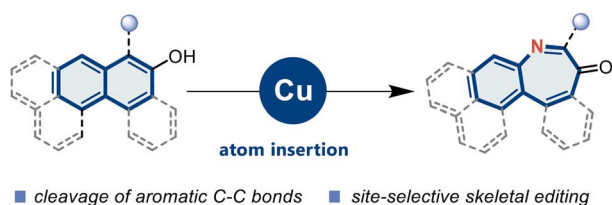
2601

### Breaking the trade-off between capacity and stability in vanadium-based zinc-ion batteries

Weikang Jiang, Kaiyue Zhu,\* Weili Xie, Zhengsen Wang, Zuqiao Ou and Weishen Yang\*



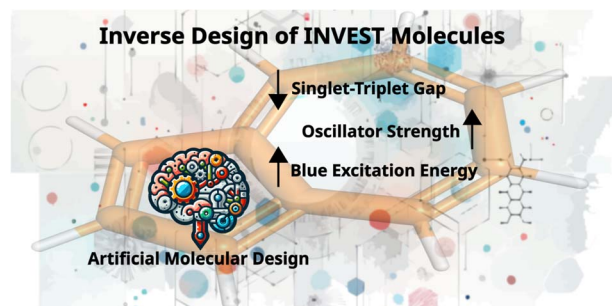
2612



### Nitrogen atom insertion into arenols to access benzazepines

Yi He, Juanjuan Wang, Tongtong Zhu, Zhaojing Zheng and Hao Wei\*

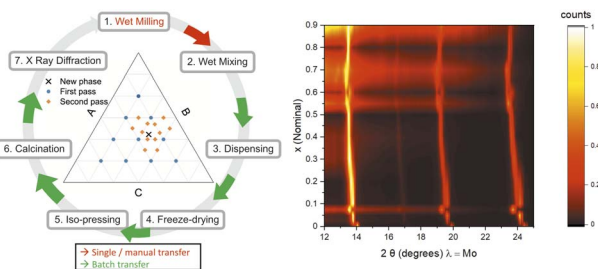
2618



### Artificial design of organic emitters via a genetic algorithm enhanced by a deep neural network

AkshatKumar Nigam, Robert Pollice,\* Pascal Friederich and Alán Aspuru-Guzik\*

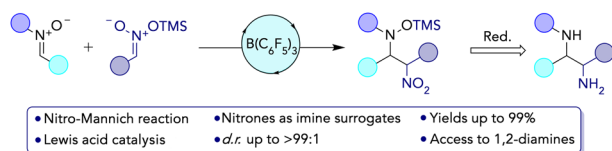
2640



### A high throughput synthetic workflow for solid state synthesis of oxides

Christopher J. Hampson, Moli P. Smith, Luca L. Arciero, Christopher M. Collins, Luke M. Daniels, Troy D. Manning, Michael W. Gaultois, John B. Claridge and Matthew J. Rosseinsky\*

2648



### An un-forgotten classic: the nitro-Mannich reaction between nitrones and silyl nitronates catalysed by B(C<sub>6</sub>F<sub>5</sub>)<sub>3</sub>

Michael G. Guerzoni, Yara van Ingen, Rasool Babaahmadi, Thomas Wirth, Emma Richards\* and Rebecca L. Melen\*

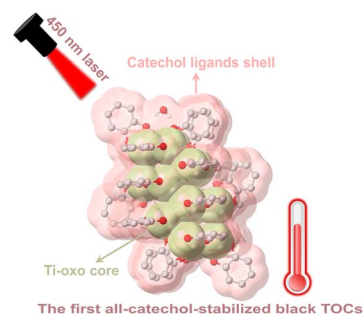


## EDGE ARTICLES

2655

**All-catecholate-stabilized black titanium-oxo clusters for efficient photothermal conversion**

Jinle Hou,\* Nahui Huang, Dinesh Acharya, Yuxin Liu, Jiaying Zhu, Jiaxin Teng, Zhi Wang, Konggang Qu, Xianxi Zhang\* and Di Sun\*



## CORRECTION

2665

**Correction: The thermodynamics and kinetics of depolymerization: what makes vinyl monomer regeneration feasible?**

Victoria Lohmann, Glen R. Jones, Nghia P. Truong and Athina Anastasaki\*

