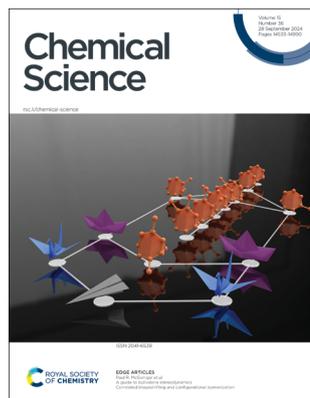


## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(36) 14533–14990 (2024)



**Cover**  
See Paul McGonigal *et al.*, pp. 14608–14617 and 14618–14624. Image reproduced by permission of Paul McGonigal from *Chem. Sci.*, 2024, **15**, 14608 and 14618.



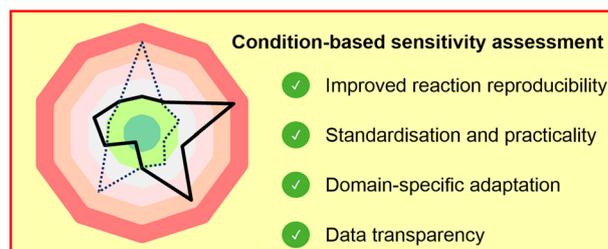
**Inside cover**  
See Shusuke Tomoshige, Minoru Ishikawa *et al.*, pp. 14625–14634. Image reproduced by permission of Shusuke Tomoshige from *Chem. Sci.*, 2024, **15**, 14625.

## PERSPECTIVE

14548

### Improving reproducibility through condition-based sensitivity assessments: application, advancement and prospect

Felix Schäfer, Lukas Lückemeier and Frank Glorius\*

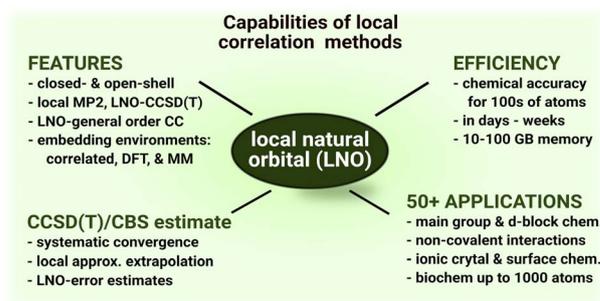


## REVIEWS

14556

### State-of-the-art local correlation methods enable affordable gold standard quantum chemistry for up to hundreds of atoms

Péter R. Nagy\*



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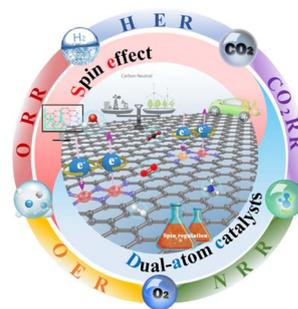
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## REVIEWS

14585

## Spin effect in dual-atom catalysts for electrocatalysis

Xiaoqin Xu and Jingqi Guan\*

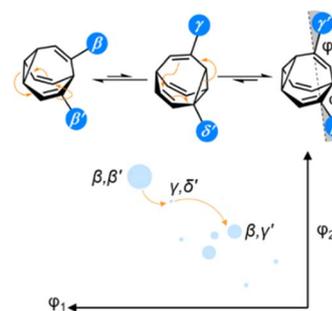


## EDGE ARTICLES

14608

## A guide to bullvalene stereodynamics

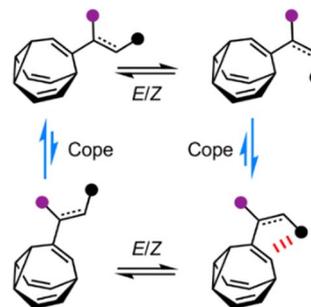
Robert A. Ives, William Maturi, Matthew T. Gill, Conor Rankine\* and Paul R. McGonigal\*



14618

## Correlated shapeshifting and configurational isomerization

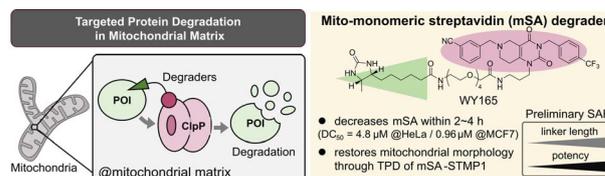
Burhan A. Hussein, William Maturi, Mary Kate Rylands, Aisha N. Bismillah, Yuzhen Wen, Juan A. Aguilar, Rabia Ayub, Conor D. Rankine and Paul R. McGonigal\*



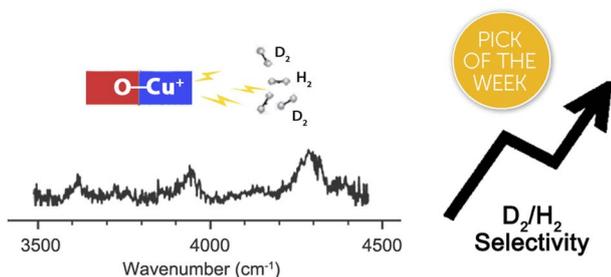
14625

## Targeted protein degradation in the mitochondrial matrix and its application to chemical control of mitochondrial morphology

Wakana Yamada, Shusuke Tomoshige,\* Sho Nakamura, Shinichi Sato and Minoru Ishikawa\*



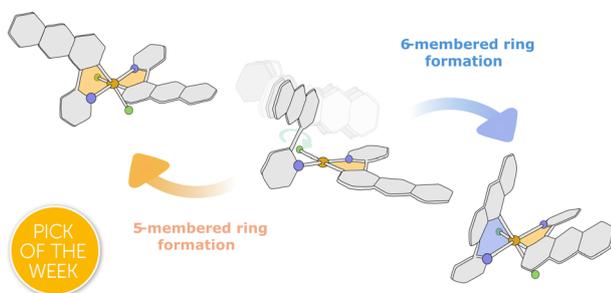
14635



### Direct evidence for ligand-enhanced activity of Cu(I) sites

Elvira Gouatieu Dongmo, Shabnam Haque, Florian Kreuter, Toshiki Wulf, Jiaye Jin,<sup>\*</sup> Ralf Tonner-Zech,<sup>\*</sup> Thomas Heine<sup>\*</sup> and Knut R. Asmis<sup>\*</sup>

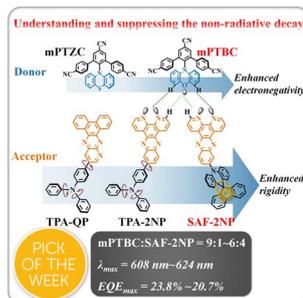
14644



### $\pi$ -Extended ligands with dual-binding behavior: hindered rotation unlocks unexpected reactivity in cyclometalated Pt complexes

Seiya Ota, Miguel A. Soto,<sup>\*</sup> Brian O. Patrick, Saeid Kamal, Francesco Lej and Mark J. MacLachlan<sup>\*</sup>

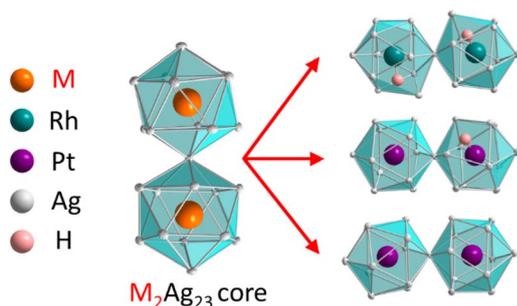
14651



### Unraveling non-radiative decay channels of exciplexes to construct efficient red emitters for organic light-emitting diodes

Heng-Yuan Zhang, Ming Zhang, Hao Zhuo, Hao-Yu Yang, Bo Han,<sup>\*</sup> Yong-Hao Zheng, Hui Wang, Hui Lin, Si-Lu Tao, Cai-Jun Zheng<sup>\*</sup> and Xiao-Hong Zhang<sup>\*</sup>

14660



### Controlled aggregation of Pt/PtH/Rh/RhH doped silver superatomic nanoclusters into 16-electron supermolecules

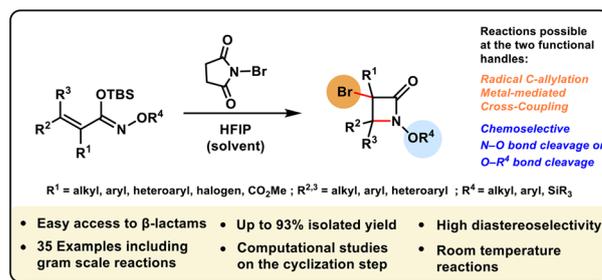
Tzu-Hao Chiu, Michael N. Pillay, Ying-Yann Wu, Yoshiki Niihori, Yuichi Negishi, Jie-Ying Chen, Yuan Jang Chen, Samia Kahlal, Jean-Yves Saillard and C. W. Liu<sup>\*</sup>



14668

### Forging structural complexity: diastereoselective synthesis of densely substituted $\beta$ -lactams with dual functional handles for enhanced core modifications

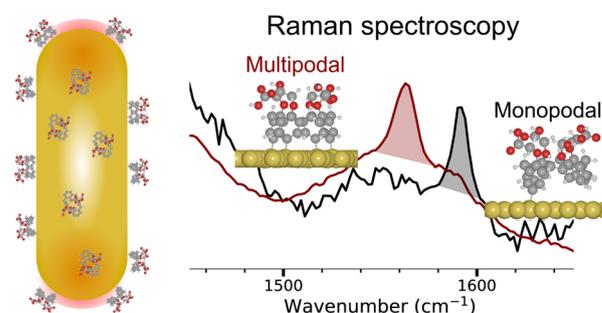
Agustin M. Rodriguez Treviño, Pierre Loch-Temzelides, Sanjay Pandiri, Justin K. Kirkland, Michael T. Davenport, Ulises Aguinaga, Muhammed Yousufuddin, Daniel H. Ess and László Kürti\*



14677

### Multipodal Au–C grafting of calix[4]arene molecules on gold nanorods

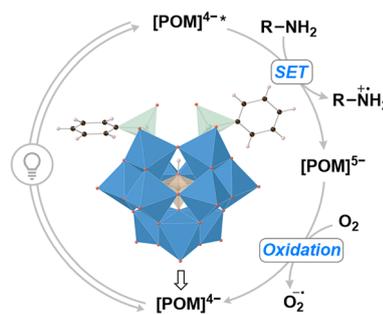
Auguste Tetenoire, Anna Omelchuk, Volodymyr Malyskyi, Ivan Jabin, Victor Lepeintre, Gilles Bruylants, Yun Luo, Arnaud Fihey, Mikaël Kepenekian\* and Corinne Lagrost\*



14685

### Organofunctionalized borotungstate polyoxometalates as tunable photocatalysts for oxidative dimerization of amines

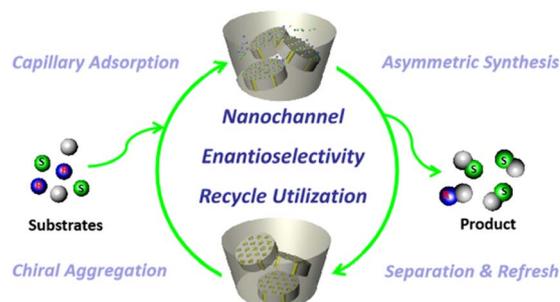
Nicole Tsang, Alexander J. Kibler, Stephen P. Argent, Hon Wai Lam,\* Kieran D. Jones\* and Graham N. Newton\*



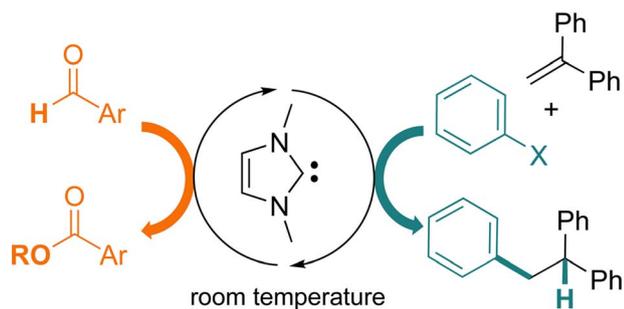
14692

### Chiral aggregates of rod-coil molecules inside nanopores as efficient nanoreactors for asymmetric synthesis

Hui-Yu Zhao, Qing Xu, Gui-Lang Liu, Yi-Rong Pei\* and Long Yi Jin\*



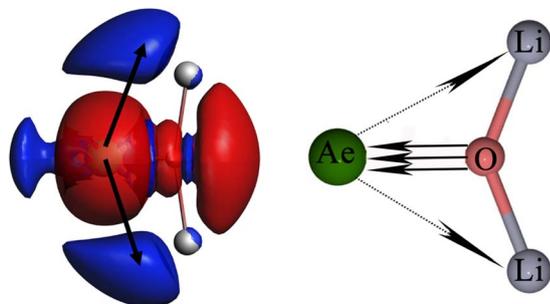
14699



### A simple N-heterocyclic carbene for the catalytic up-conversion of aldehydes into stoichiometric super electron donors

Nahrata Assani, Ludivine Delfau, Preslav Smits, Sébastien Redon, Youssef Kabri, Eder Tomás-Mendivil, Patrice Vanelle, David Martin\* and Julie Broggi\*

14705



### Unusual quadruple bonds featuring collective interaction-type $\sigma$ bonds between first octal-row atoms in the alkaline-earth compounds $AeOLi_2$ ( $Ae = Be-Ba$ )

Li-Juan Cui, Yu-Qian Liu, Sudip Pan,\* Zhong-Hua Cui\* and Gernot Frenking\*

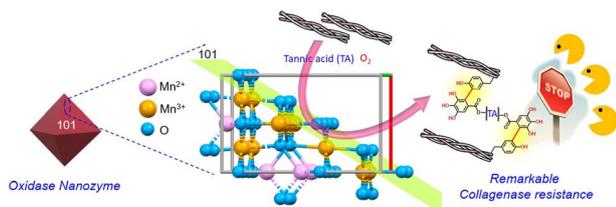
14721



### A compact chemically driven [2]catenane rotary motor operated through alternate pumping and discharging

Anquan Li, Zhenglin Du, Shilong Zhang, Jialin Xie, Xia Li, Qing Chen, Yisong Tang, Jiawen Chen and Kelong Zhu\*

14726



### Expanding limits of artificial enzymes: unprecedented catalysis by an oxidase nanozyme in activating a structural protein for covalent crosslinking and conferring remarkable proteolytic resistance

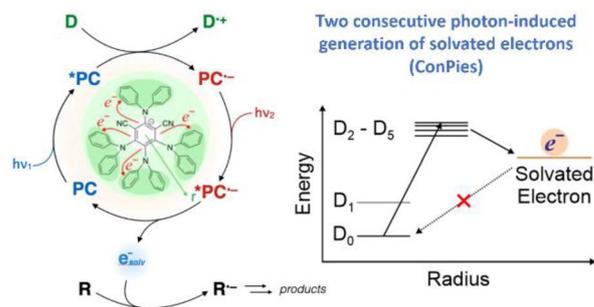
Adarsh P. Fatrekar, Rasmi V. Morajkar and Amit A. Vernekar\*



14739

### Organic super-reducing photocatalysts generate solvated electrons *via* two consecutive photon induced processes

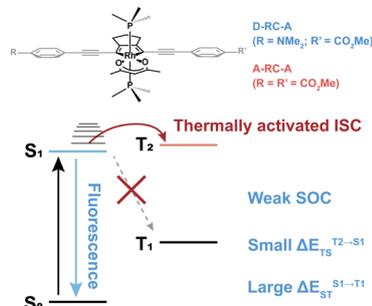
Marco Villa, Andrea Fermi, Francesco Calogero, Xia Wu, Andrea Gualandi, Pier Giorgio Cozzi, Alessandro Troisi,\* Barbara Ventura\* and Paola Ceroni\*



14746

### Ultrafast photophysics of *para*-substituted 2,5-bis(arylethynyl) rhodacyclopentadienes: thermally activated intersystem crossing

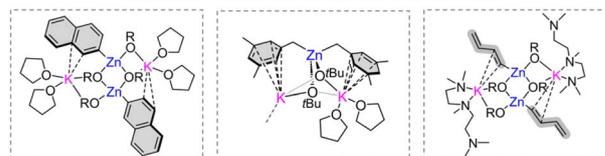
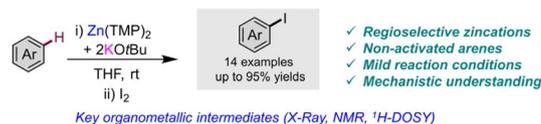
Zilong Guo, Yaxin Wang, Julia Heitmüller, Carolin Sieck, Andreas Prüfer, Philipp Ralle, Andreas Steffen, Petr Henke, Peter R. Ogilby,\* Todd B. Marder,\* Xiaonan Ma\* and Tobias Brixner\*



14757

### Combining two relatively weak bases ( $Zn(TMP)_2$ and $KOtBu$ ) for the regioselective metalation of non-activated arenes and heteroarenes

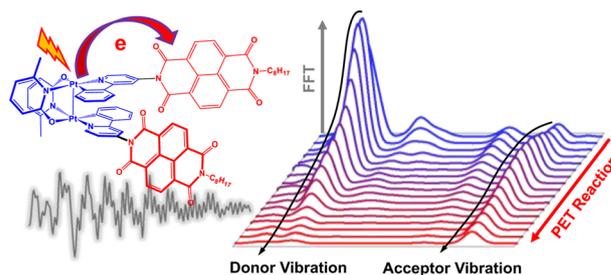
Neil R. Judge and Eva Hevia\*



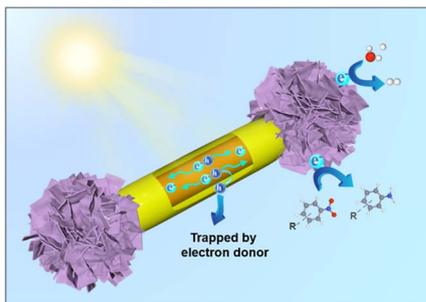
14766

### Real-time capture of nuclear motions influencing photoinduced electron transfer

Pyosang Kim,\* Subhangi Roy, Andrew J. S. Valentine, Xiaolin Liu, Sarah Kromer, Tae Wu Kim, Xiaosong Li,\* Felix N. Castellano\* and Lin X. Chen\*



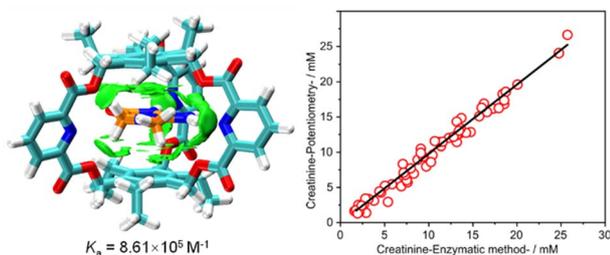
14778



### Customizing dumbbell-shaped heterostructured artificial photosystems steering versatile photoredox catalysis

Peng Su, Xian Yan and Fang-Xing Xiao\*

14791

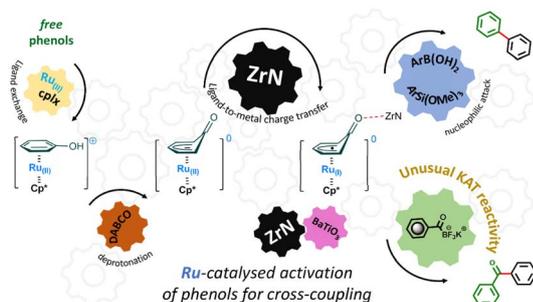


Accurate analysis of creatinine for real samples

### An *endo*-functionalized molecular cage for selective potentiometric determination of creatinine

Yu Lu, Song-Meng Wang, Sui-Sui He, Qicheng Huang, Cheng-Da Zhao, Shan Yu, Wei Jiang, Huan Yao,\* Li-Li Wang\* and Liu-Pan Yang\*

14798

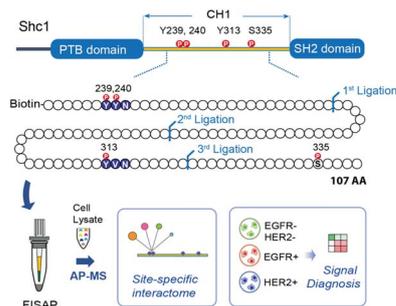


Ru-catalysed activation of phenols for cross-coupling

### Ru-catalyzed activation of free phenols in a one-step Suzuki–Miyaura cross-coupling under mechanochemical conditions

Satenik Mkrtchyan, Michał Jakubczyk, Sehrish Sarfaraz, Khurshid Ayub and Viktor O. Iaroshenko\*

14806



### Dissecting phospho-motif-dependent Shc1 interactome using long synthetic protein fragments

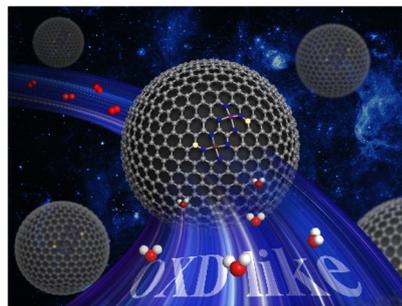
Peizhong Chen, Xiong Chen, Xiaolei Song, An He, Yong Zheng,\* Xuechen Li\* and Ruijun Tian\*



14816

### Theory-guided design of S-doped Fe/Co dual-atom nanozymes for highly efficient oxidase mimics

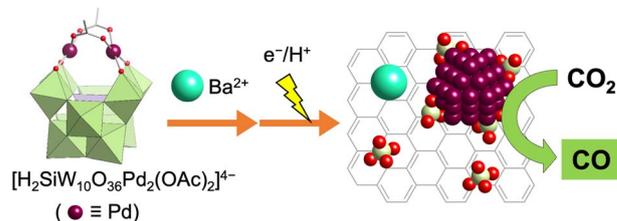
Huan Cheng, Yanyue Chen, Mingjia Liu, Hongling Tao, Lu Chen, Fupeng Wang, Long Huang, Jian Tang,\* Tong Yang\* and Rong Hu\*



14829

### Pd-incorporated polyoxometalate catalysts for electrochemical CO<sub>2</sub> reduction

Kimitake Kawakami, Tomohiro Yabe, Fumiaki Amano, Kazuya Yamaguchi and Kosuke Suzuki\*

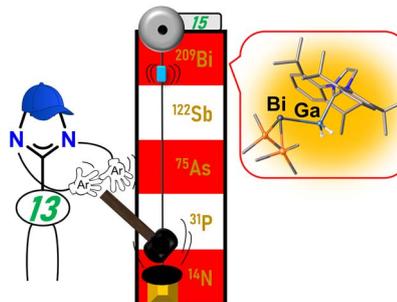


- ✓ Selective and stable CO production
- ✓ Control of electrochemical CO<sub>2</sub>RR performance through manipulation of counteranions

14837

### Synthesis of bismuthanyl-substituted monomeric triel hydrides

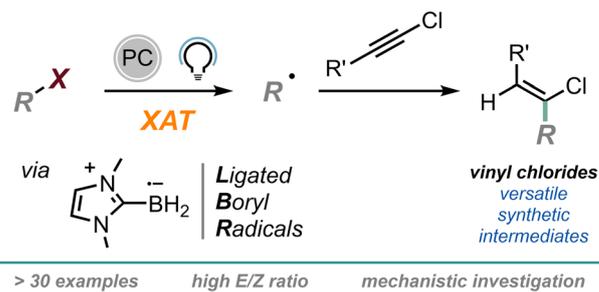
Robert Szlosek, Christian Marquardt, Oliver Hegen, Gábor Balázs, Christoph Riesinger, Alexey Y. Timoshkin and Manfred Scheer\*



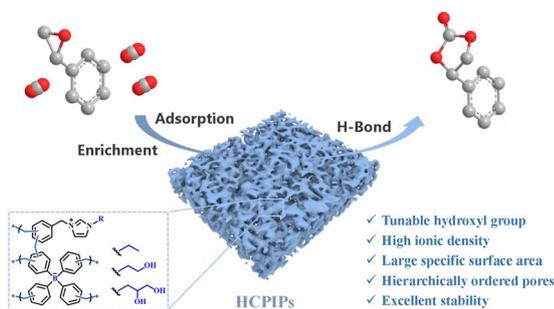
14844

### Visible light-induced halogen-atom transfer by N-heterocyclic carbene-ligated boryl radicals for diastereoselective C(sp<sup>3</sup>)-C(sp<sup>2</sup>) bond formation

Luca Capaldo,\* Ting Wan, Robin Mulder, Jonas Djossou and Timothy Noël\*



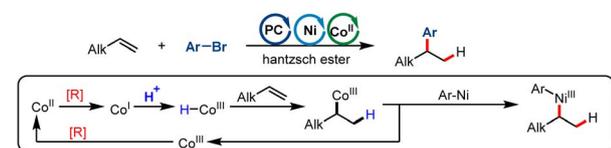
14851



### Non-cationic hyper-crosslinked ionic polymers with hierarchically ordered porous structures: facile synthesis and applications for highly efficient CO<sub>2</sub> capture and conversion

Bihua Chen, Junfeng Zeng, Shiguo Zhang\* and Yan Zhang\*

14865

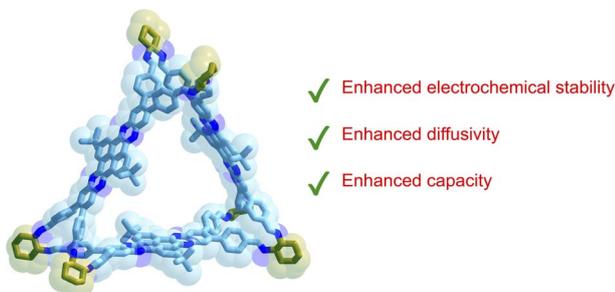


- First example of photoinduced MHAT via reductive route intercepting an organometallic coreactant
- Building quaternary carbons
- Unique Markovnikov selectivity
- Si-H free
- Oxidant free
- High catalytic efficiency

### Photoinduced Co/Ni-cocatalyzed Markovnikov hydroarylation of unactivated olefins with aryl bromides

Hong-Chao Liu, Xin-Yu Xu, Siyuan Tang, Jiawei Bao, Yu-Zhao Wang, Yiliang Chen, Xinya Han,\* Yong-Min Liang\* and Kui Zhang\*

14872

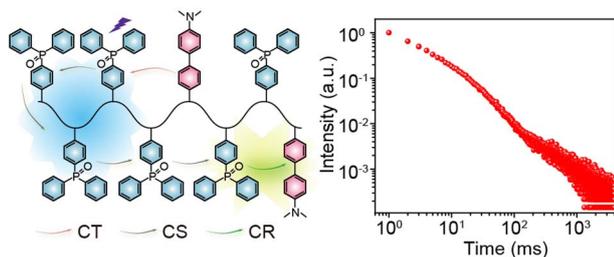


### A redox-active organic cage as a cathode material with improved electrochemical performance

Saibal Bera, Nicolas Goujon, Manuel Melle-Franco, David Mecerreyes\* and Aurelio Mateo-Alonso\*

14880

### Single-Component Exciplex Organic Long-Persistent Luminescence



### Highly stable color-tunable organic long-persistent luminescence from a single-component exciplex copolymer for *in vitro* antibacterial

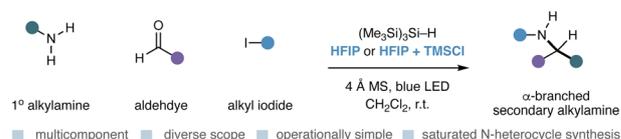
Hui Li,\* Xiaoye Li, Haoran Su, Shuman Zhang, Cheng Tan, Cheng Chen, Xin Zhang, Jiani Huang, Jie Gu, Huanhuan Li, Gaozhan Xie, Heng Dong,\* Runfeng Chen and Ye Tao\*



14888

### Modular synthesis of $\alpha$ -branched secondary alkylamines via visible-light-mediated carbonyl alkylative amination

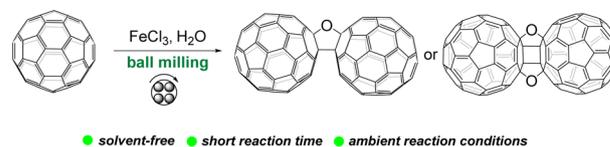
Milo A. Smith, Ryan J. D. Kang, Roopender Kumar, Biswarup Roy and Matthew J. Gaunt\*



14899

### Unexpected and divergent mechanosynthesis of furanoid-bridged fullerene dimers $\text{C}_{120}\text{O}$ and $\text{C}_{120}\text{O}_2$

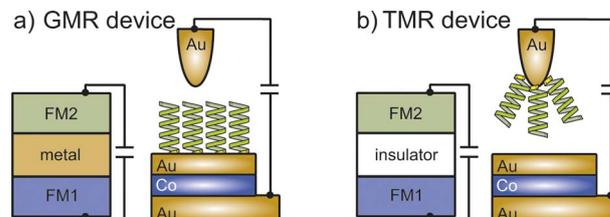
Gang Shao, Yuan-Yuan Liu, Chuang Niu, Zheng-Chun Yin, Shi-Qi Ye, Yang-Rong Yao, Muqing Chen, Jun-Shen Chen, Xu-Ling Xia, Shangfeng Yang\* and Guan-Wu Wang\*



14905

### The mechanism of the molecular CISS effect in chiral nano-junctions

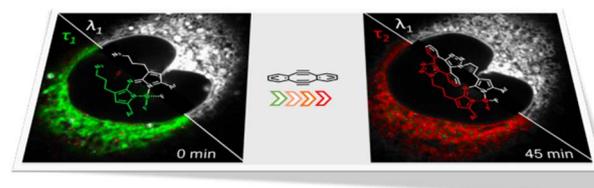
Thi Ngoc Ha Nguyen, Georgeta Salvan, Olav Hellwig, Yossi Paltiel, Lech Tomasz Baczewski and Christoph Tegenkamp\*



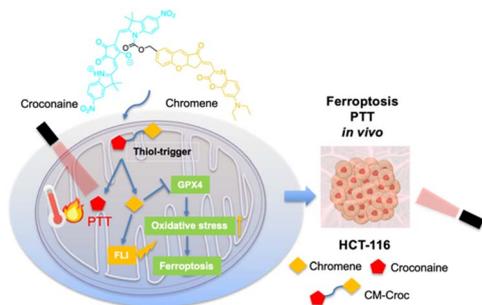
14913

### Observing bioorthogonal macrocyclizations in the nuclear envelope of live cells using on/on fluorescence lifetime microscopy

Sebastian Pim, Anaïs C. Bourgès, Dan Wu, Gonzalo Durán-Sampedro, Massimiliano Garre and Donal F. O'Shea\*



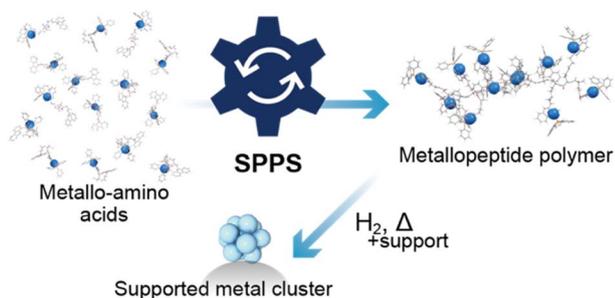
14924



### A thiol-triggered croconaine–chromene integration to induce ferroptosis and photothermal synergistic efficient tumor ablation

Xinya Niu, He Yang, Xingkang Wu, Fangjun Huo, Kaiqing Ma\* and Caixia Yin\*

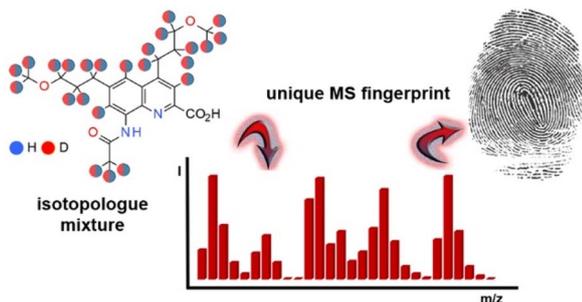
14931



### Synthesis of atom-precise supported metal clusters via solid-phase peptide synthesis

Takane Imaoka,\* Nanami Antoku, Yusuke Narita, Kazuki Nishiyama, Kenji Takada, Shogo Saito, Masayoshi Tanaka, Mina Okochi, Miftakul Huda, Makoto Tanabe, Wang-Jae Chun and Kimihisa Yamamoto\*

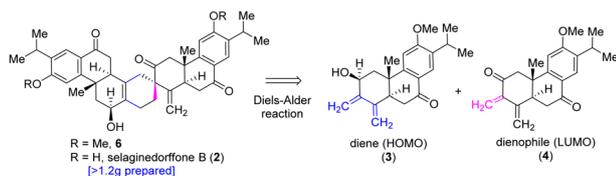
14938



### High density information storage through isotope ratio encoding

Petra Sőregi, Márton Zwillinger, Lajos Vágó, Márton Csékei\* and Andras Kotschy\*

14946



### Biomimetic total synthesis of the reported structure of (+)-selaginedorffone B

Sourav Kundu, Debdeep Jana, Nilangshu Mandal, Ayan Mondal, Ranjit Murmu, Nanda Kishore Roy, Ayan Datta\* and Alakesh Bisai\*

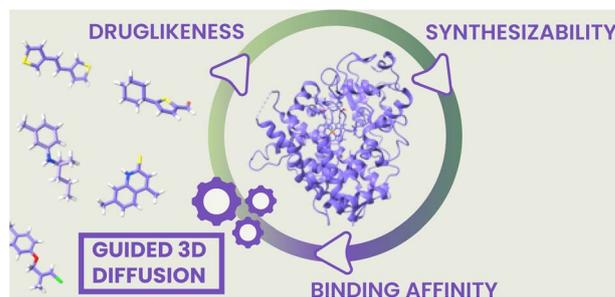


## EDGE ARTICLES

14954

**PILOT: equivariant diffusion for pocket-conditioned *de novo* ligand generation with multi-objective guidance via importance sampling**

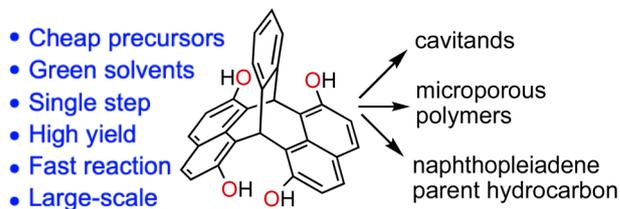
Julian Cremer,\* Tuan Le,\* Frank Noé, Djork-Arné Clevert and Kristof T. Schütt



14968

**Triptycene-like naphthopleiadene as a readily accessible scaffold for supramolecular and materials chemistry**

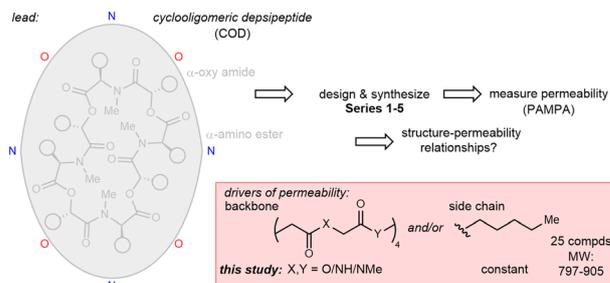
Md Khairul Amin, Chunchun Ye, Shuhua Pang, Yuancheng Liu, Dominic Taylor, Gary S. Nichol and Neil B. McKeown\*



14977

**The backbone constitution drives passive permeability independent of side chains in depsipeptide and peptide macrocycles inspired by *ent*-verticilide**

Madelaine P. Thorpe, Abigail N. Smith, Daniel J. Blackwell, Corey R. Hopkins, Bjorn C. Knollmann, Wendell S. Akers and Jeffrey N. Johnston\*



## CORRECTION

14988

**Correction: Re-pairing DNA: binding of a ruthenium phi complex to a double mismatch**

Tayler D. Prieto Otoyá, Kane T. McQuaid, Neil G. Paterson, David J. Cardin, Andrew Kellett and Christine J. Cardin\*

