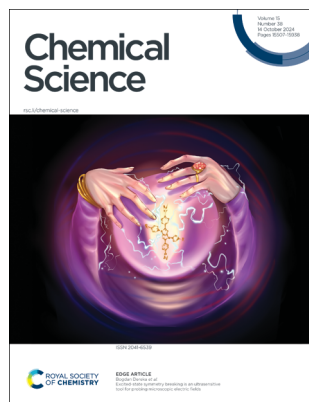


## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(38) 15507–15938 (2024)



**Cover**  
See Bogdan Dereka *et al.*, pp. 15565–15576. Image reproduced by permission of Bogdan Dereka from *Chem. Sci.*, 2024, **15**, 15565. Artwork created by Zlata Korotchenko.



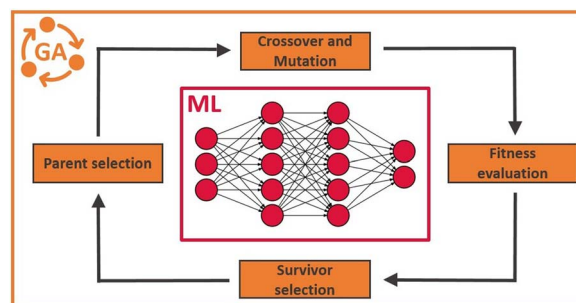
**Inside cover**  
See Dean J. Tantillo *et al.*, pp. 15577–15587. Image reproduced by permission of Dean J. Tantillo from *Chem. Sci.*, 2024, **15**, 15577.

## PERSPECTIVE

15522

### Augmenting genetic algorithms with machine learning for inverse molecular design

Hannes Kneiding and David Balcells\*

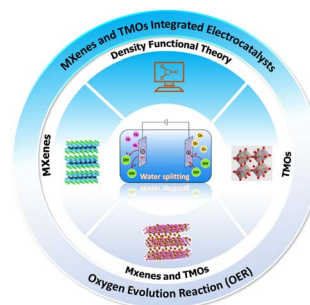


## REVIEW

15540

### Integrated MXene and metal oxide electrocatalysts for the oxygen evolution reaction: synthesis, mechanisms, and advances

Muhammad Nazim Lakhan, Abdul Hanan, Yuan Wang, Hiang Kwee Lee and Hamidreza Arandiyani\*



**GOLD  
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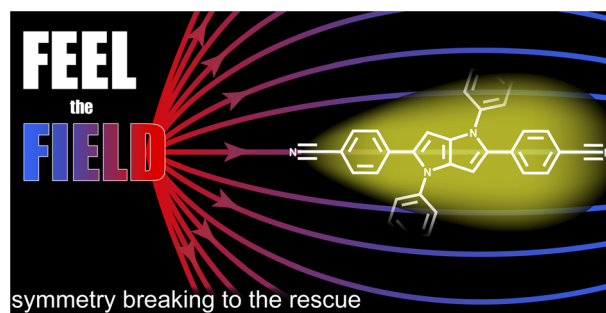
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15565

### Excited-state symmetry breaking is an ultrasensitive tool for probing microscopic electric fields

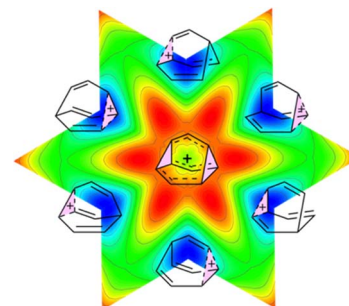
Bogdan Dereka,\* Nikhil Maroli, Yevgen M. Poronik, Daniel T. Gryko and Alexei A. Kananenka



15577

### Revisiting a classic carbocation – DFT, coupled-cluster, and *ab initio* molecular dynamics computations on barbaralyl cation formation and rearrangements

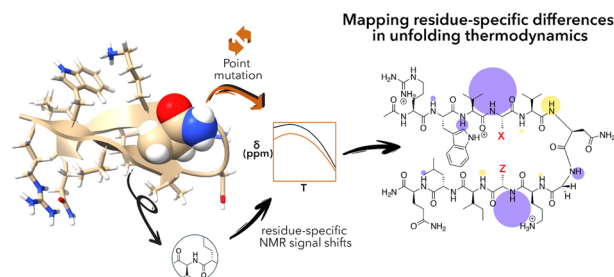
Wentao Guo, Wang-Yeuk Kong and Dean J. Tantillo\*



15588

### Probing the non-covalent forces key to the thermodynamics of $\beta$ -hairpin unfolding

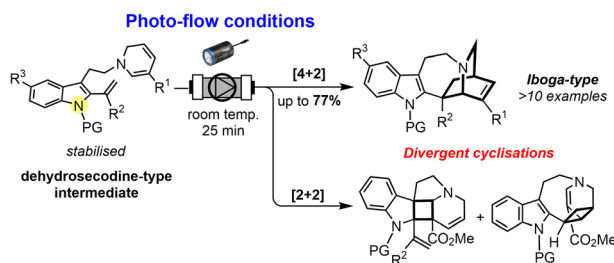
Thien H. Tran, Priyanka Prusty, Meghan Ricciardi, Christopher R. Travis, Marcey L. Waters and Bruce C. Gibb\*



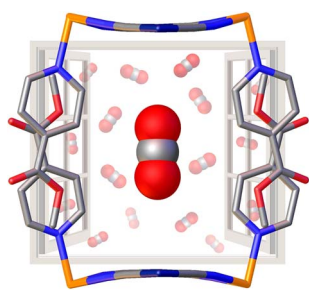
15599

### Direct photochemical intramolecular [4 + 2] cycloadditions of dehydrosecodine-type substrates for the synthesis of the *iboga*-type scaffold and divergent [2 + 2] cycloadditions employing micro-flow system

Gavin Tay, Soushi Nishimura and Hiroki Oguri\*



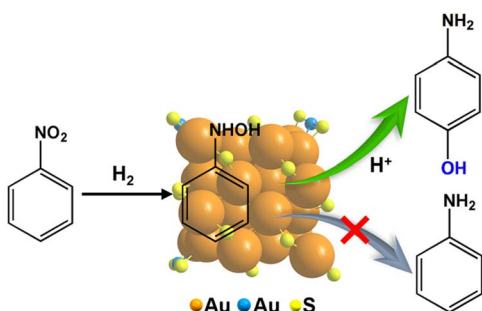
15610

CO<sub>2</sub>-gated magnetic transition

### CO<sub>2</sub>-actuated spin transition tuning in an interdigitated Hofmann-type coordination polymer

Abhik Paul, Wataru Kosaka, Bhart Kumar, Dibya Jyoti Mondal, Hitoshi Miyasaka\* and Sanjit Konar\*

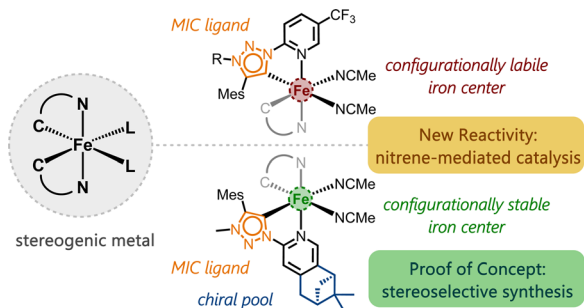
15617



### Exclusive catalytic hydrogenation of nitrobenzene toward *p*-aminophenol over atomically precise Au<sub>36</sub>(SR)<sub>24</sub> clusters

Jinzhi Lu, Kun Tang, Guodong Qi, Chao Juan, Jun Xu, Zhenfeng Cai, Dan Li,\* Xiao Cai, Xu Liu, Mingyang Chen,\* Weiping Ding and Yan Zhu\*

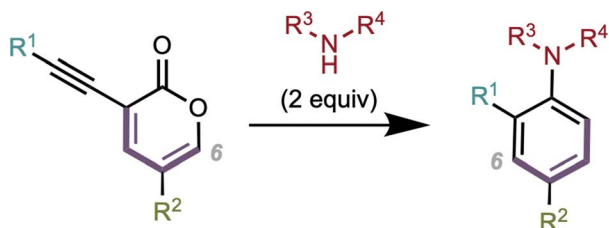
15625



### Stereogenic-at-iron mesoionic carbene complex for enantioselective C–H amidation

Nemrud Demirel, Mahiob Dawor, Greta Nadler, Sergei I. Ivlev and Eric Meggers\*

15632



### Modular synthesis of aryl amines from 3-alkynyl-2-pyrones

Kristen E. Gardner, Louis de Lescure, Melissa A. Hardy, Jin Tan, Matthew S. Sigman,\* Robert S. Paton\* and Richmond Sarpong\*

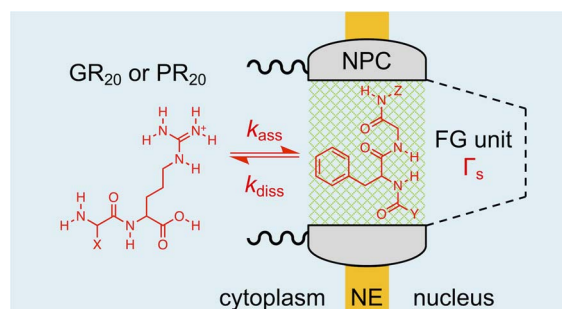
• "no-metal-added" • >30 examples • aryl amine synthesis  
• unusual transformation supported by DFT



15639

### Nanoscale interactions of arginine-containing dipeptide repeats with nuclear pore complexes as measured by transient scanning electrochemical microscopy

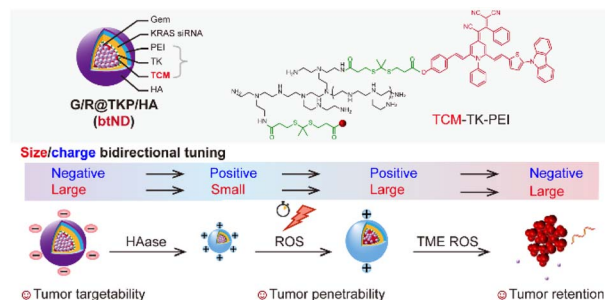
Siao-Han Huang, Moghitha Parandhaman, Manu Jyothi Ravi, Donald C. Janda and Shigeru Amemiya\*



15647

### Cascade-responsive size/charge bidirectional-tunable nanodelivery penetrates pancreatic tumor barriers

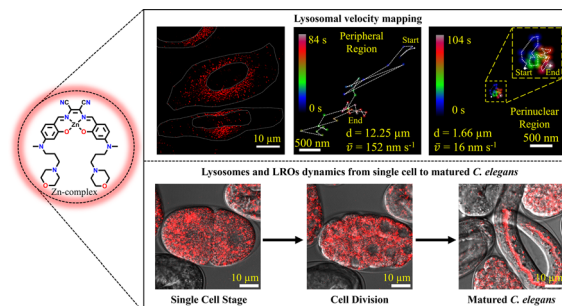
Yiqi Shi, Jinghan Liao, Cuiyun Zhang, Qi Wu, Shanshan Hu, Ting Yang, Jihong Liu, Zhirong Zhu, Wei-Hong Zhu and Qi Wang\*



15659

### A zinc metal complex as an NIR emissive probe for real-time dynamics and *in vivo* embryogenic evolution of lysosomes using super-resolution microscopy

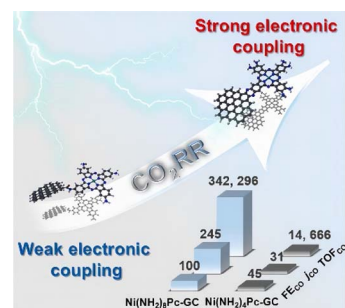
Abdul Salam, Kush Kaushik, Bodhidipra Mukherjee, Farhan Anjum, Goraksha T. Sapkal, Shagun Sharma, Richa Garg and Chayan Kanti Nandi\*



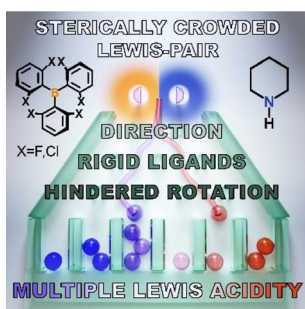
15670

### Graphite conjugated nickel phthalocyanine for efficient CO<sub>2</sub> electroreduction and Zn–CO<sub>2</sub> batteries

Jingwei Han, Qiang Xu, Fengkun Tian, Hai Sun, Yuanyuan Qi, Guodong Zhang, Jun-Sheng Qin and Heng Rao\*



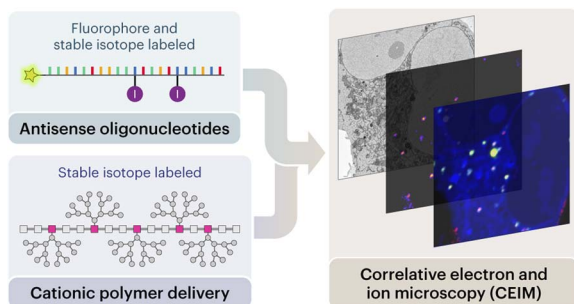
15679



### Illuminating the multiple Lewis acidity of triarylboranes *via* atropisomeric dative adducts

Benjámín Kovács, Tamás Földes, Márk Szabó, Éva Dorkó, Bianka Kótai, Gergely Laczkó, Tamás Holczbauer, Attila Domján,\* Imre Pápai\* and Tibor Soós\*

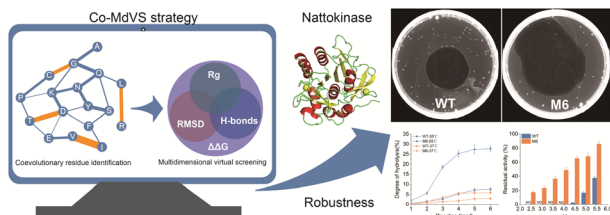
15690



### High-resolution visualisation of antisense oligonucleotide release from polymers in cells

Jessica J. King, Kai Chen, Cameron W. Evans, Marck Norret, Ruba Almasri, Nathan J. Pavlos, Henry YL. Hui, Qiongxiang Lin, Udit Bhatt, Stephen G. Young, Nicole M. Smith, Mehran Nikan, Clive A. Prestidge, Haibo Jiang\* and K. Swaminathan Iyer\*

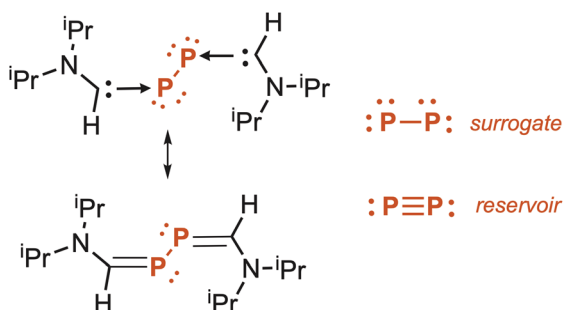
15698



### Precise redesign for improving enzyme robustness based on coevolutionary analysis and multidimensional virtual screening

Jie Luo, Chenshuo Song, Wenjing Cui, Qiong Wang, Zhemin Zhou\* and Laichuang Han\*

15713



### A carbene-stabilized diphosphorus: a triple-bonded diphosphorus ( $P\equiv P$ ) and a bis(phosphinidene) ( $P=P$ ) transfer agent

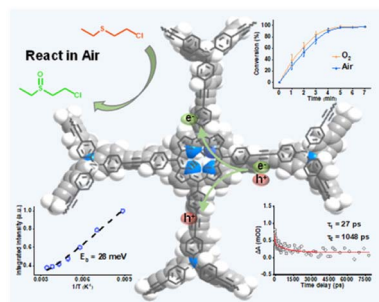
Joseph S. Yoon, Mehdi Abdellaoui, Milan Gembicky and Guy Bertrand\*



15717

### Exclusive generation of a superoxide radical by a porous aromatic framework for fast photocatalytic decontamination of mustard gas simulant in room air

Jian Song, Hengtao Lei, Yuhui Zhai, Zilong Dou, Yongyue Ding, Xueyan Han, Fengchao Cui, Yuyang Tian\* and Guangshan Zhu\*



15725

### $N_2H_4Zn(HC_3N_3O_3)$ : exceptionally strong second harmonic generation and ultra-long phosphorescence

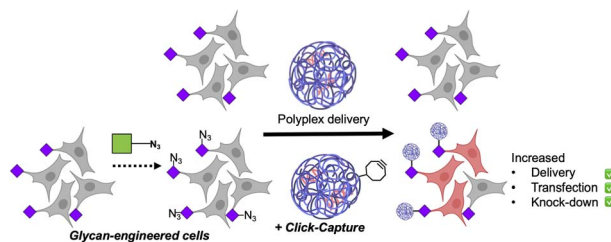
Can Yang, Yuwei Kang, Xuefei Wang, Jie Gou, Yi Xiong, Zece Zhu, Ling Chen\* and Qi Wu\*



15731

### Covalent recruitment of polymers and nanoparticles onto glycan-engineered cells enhances gene delivery during short exposure

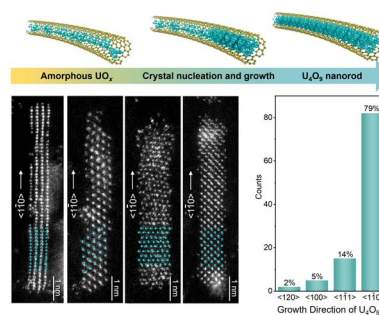
Qiao Tang, Ruben M. F. Tomás and Matthew I. Gibson\*



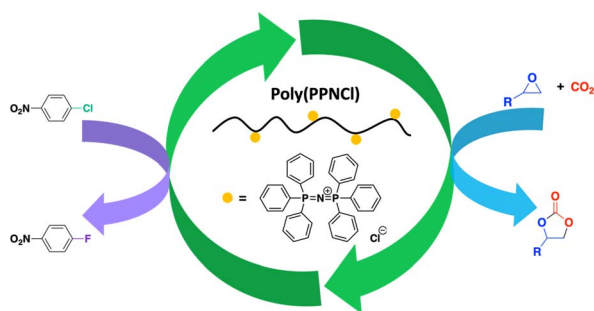
15737

### Directional growth and reconstruction of ultrafine uranium oxide nanorods within single-walled carbon nanotubes

Luyao Zhang, Kun Wang, Xin Zhao, Guoping Yang, Yulong Jiang and Feng Yang\*



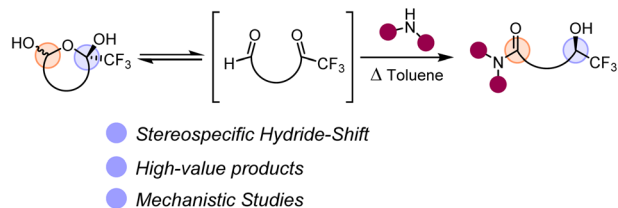
15745



### Polymeric bis(triphenylphosphine)iminium chloride as a recyclable catalyst

Ziwei Xu, Meng Wang and Michael P. Shaver\*

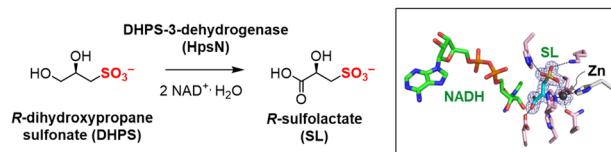
15751



### Diastereoselective hydride transfer enables a synthesis of chiral 1,5-carboxamido-trifluoromethylcarbinols

Roberto Tinelli, Manuel Schupp, Immo Klose, Saad Shaaban, Boris Maryasin, Leticia González and Nuno Maulide\*

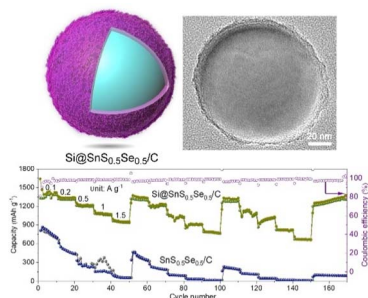
15757



### Structural and kinetic insights into the stereospecific oxidation of R-2,3-dihydroxypropanesulfonate by DHPS-3-dehydrogenase from *Cupriavidus pinatubonensis*

Laura Burchill, Arashdeep Kaur, Artur Nastasovici, Mihwa Lee\* and Spencer J. Williams\*

15769



### Rationally engineering a binary SnS<sub>0.5</sub>Se<sub>0.5</sub>/carbon nest-coated Si nanosphere for a high-performance lithium-ion battery anode

Hui Zhang, Kehao Tao, Xiangbing Zeng, Chengbing Chen, Yajun Zhu, Tianli Han, Jinjin Li\* and Jinyun Liu\*

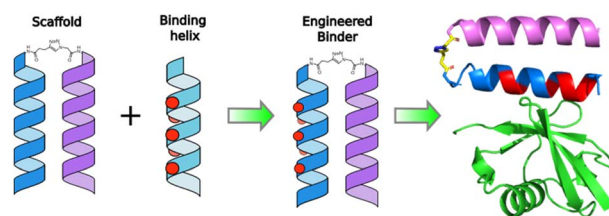




15776

**An engineered ubiquitin binding coiled coil peptide**

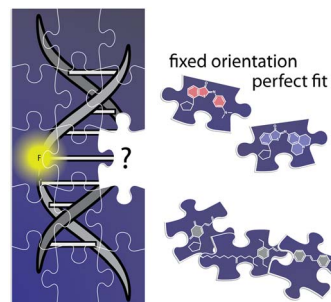
Pernille Vosbein, Paula Paredes Vergara, Danny T. Huang and Andrew R. Thomson\*



15783

**Dark times: iminothioindoxyl-C-nucleoside fluorescence quenchers with defined location and minimal perturbation in DNA**

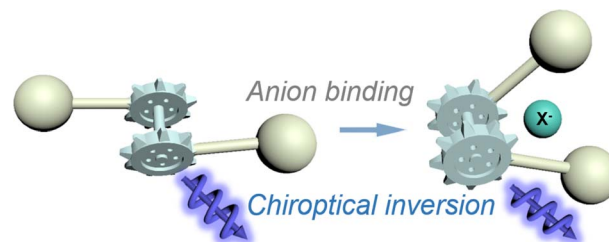
Larita Luma, Judith C. Pursteiner, Tobias Fischer, Rainer Hegger, Irene Burghardt,\* Josef Wachtveitl\* and Alexander Heckel\*



15790

**A photoactivated chiral molecular clamp rotated by selective anion binding**

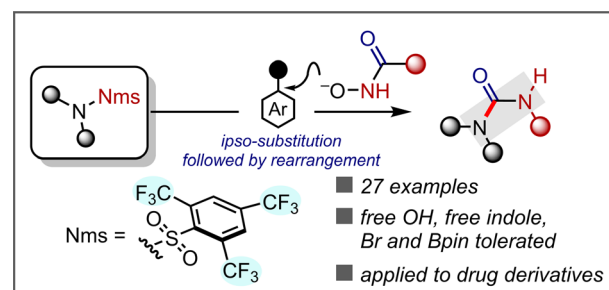
Yiping Liu, Aiyou Hao and Pengyao Xing\*



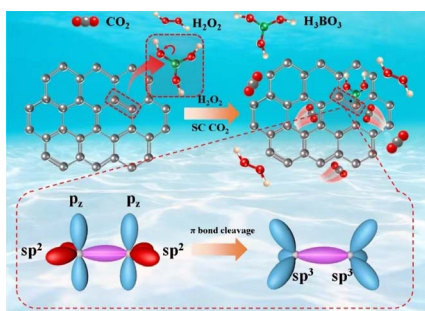
15799

**Deprotective Lossen rearrangement: a direct and general transformation of Nms-amides to unsymmetrical ureas**

Philipp Spieß, Jakub Brzeškiewicz and Nuno Maulide\*



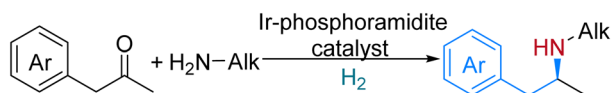
15804



### Introduction of the $-\text{B}(\text{OH})_2$ group into a graphene motif for $p_z$ orbital removal and ferromagnetic modulation

Di Zhang, Bo Gao, Yuqi Ouyang, Song Xu,<sup>\*</sup> Qingyong Tian, Wenzhuo Wu and Qun Xu<sup>\*</sup>

15811

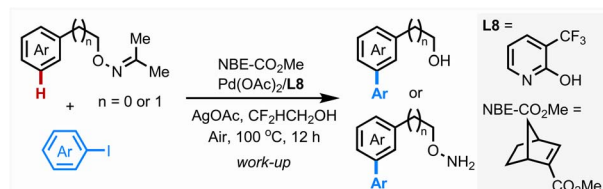


- ★ Low cata. loading (0.03 mol%)
- ★ Additive-free conditions
- ★ Broad ketone substrate scope
- ★ Alkylamine sources
- ★ Ligands with 3 blocking planes
- ★ Multiple drug synthesis

### Direct synthesis of chiral $\beta$ -arylamines via additive-free asymmetric reductive amination enabled by tunable bulky phosphoramidite ligands

Jing Wang, Wenji Wang, Haizhou Huang, Zhiqing Ma and Mingxin Chang<sup>\*</sup>

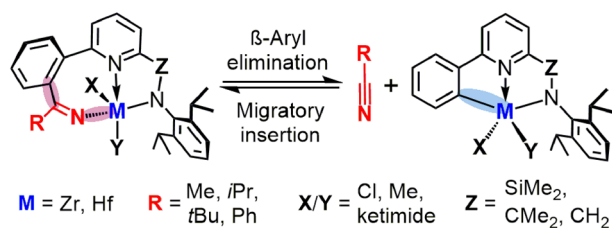
15819



### *meta*-C–H functionalization of phenylethyl and benzylic alcohol derivatives via Pd/NBE relay catalysis

Hua-Chen Shen, Jian-Jun Li, Peng Wang<sup>\*</sup> and Jin-Quan Yu<sup>\*</sup>

15825



### Reversible C–C bond formation in group 4 metal complexes: nitrile extrusion via $\beta$ -aryl elimination

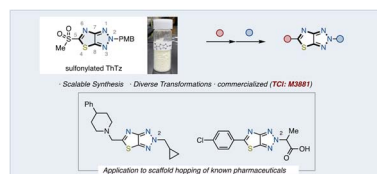
Pavel S. Kulyabin, Georgy P. Goryunov, Andrei N. Iashin, Dmitry Y. Mladentsev, Dmitry V. Uborsky, Christian Ehm, Jo Ann M. Canich, John R. Hagadorn and Alexander Z. Voskoboynikov<sup>\*</sup>



15835

## 2H-Thiazolo[4,5-d][1,2,3]triazole: synthesis, functionalization, and application in scaffold-hopping

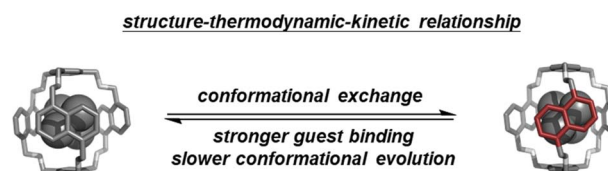
Ryuya Miyazaki, Fumito Takada, Takunari Kikuchi, Yuya Oguro, Makoto Kamata, Takafumi Yukawa, Kenta Kato, Kei Muto\* and Junichiro Yamaguchi\*



15841

## Kinetic–thermodynamic correlation of conformational changes in ammonium complexes of a flexible naphthocage

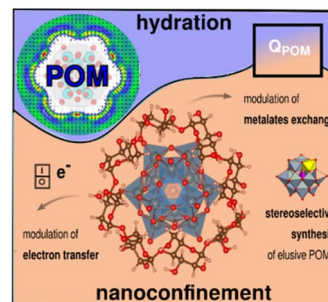
Shan He, Mao Quan, Liu-Pan Yang, Ho Yu Au-Yeung\* and Wei Jiang



15849

## Nanoconfinement of polyoxometalates in cyclodextrin: computational inspections of the binding affinity and experimental demonstrations of reactivity modulation

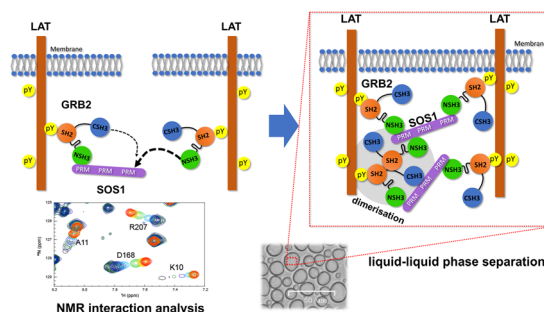
Mireia Segado-Centellas,\* Clément Falaise,\* Nathalie Leclerc, Gabrielle Mpacko Priso, Mohamed Haouas, Emmanuel Cadot and Carles Bo



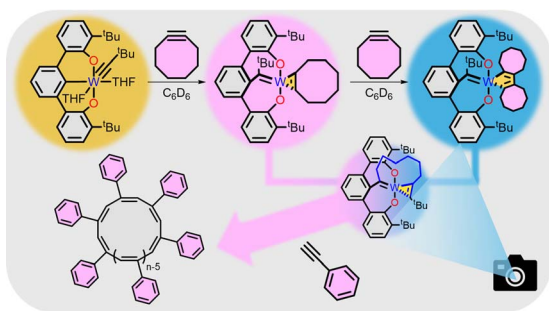
15858

## Different molecular recognition by three domains of the full-length GRB2 to SOS1 proline-rich motifs and EGFR phosphorylated sites

Keita Tateno, Takami Ando, Maako Tabata, Haruka Sugawara, Toshifumi Hayashi, Sangya Yu, Sayeesh PM, Kohsuke Inomata, Tsutomu Mikawa, Yutaka Ito\* and Teppei Ikeya\*



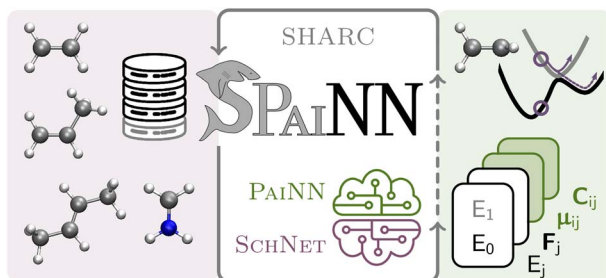
15873



### Snapshot of cyclooctyne ring-opening to a tethered alkydene cyclic polymer catalyst

Javier M. Hurst, Rinku Yadav, Parker T. Boeck, Ion Ghiviriga, ChristiAnna L. Brantley, Łukasz Dobrzycki and Adam S. Veige\*

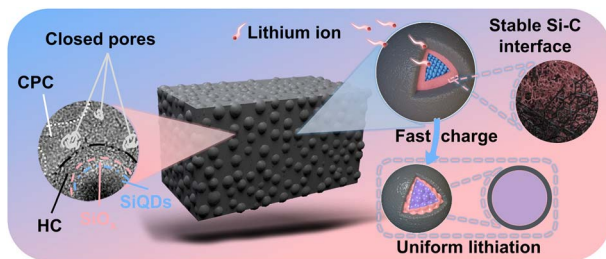
15880



### SPAINN: equivariant message passing for excited-state nonadiabatic molecular dynamics

Sascha Mausenberger, Carolin Müller,\* Alexandre Tkatchenko, Philipp Marquetand, Leticia González and Julia Westermayr\*

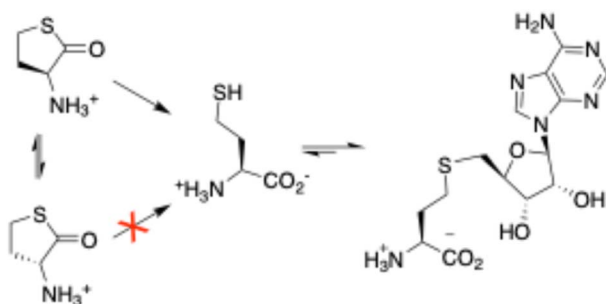
15891



### Alleviating the volume expansion of silicon anodes by constructing a high-strength ordered multidimensional encapsulation structure

Yun Yu, Haiqiang Gong, Xinyou He, Lei Ming,\* Xiaowei Wang\* and Xing Ou\*

15900



### Enzymatic synthesis of *S*-adenosyl-*L*-homocysteine and its nucleoside analogs from racemic homocysteine thiolactone

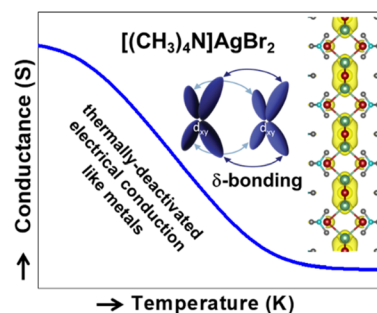
Xiaojin Wen, Viviane Leopold and Florian P. Seebeck\*



15907

### Ultralow thermal conductivity and thermally-deactivated electrical transport in a 1D silver array with alternating $\delta$ -bonds

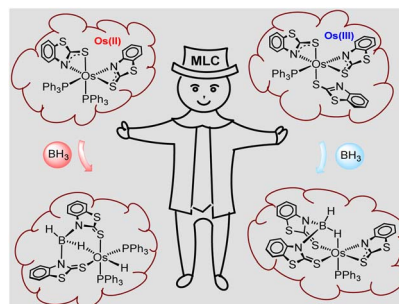
Nahid Hassan, Suneetha Nagaraja, Sauvik Saha, Kartick Tarafder and Nirmalya Ballav\*



15913

### Quantifying variation in cooperative B–H bond activations using Os(II) and Os(III) $\kappa^2$ -N,S-chelated complexes: same, but different

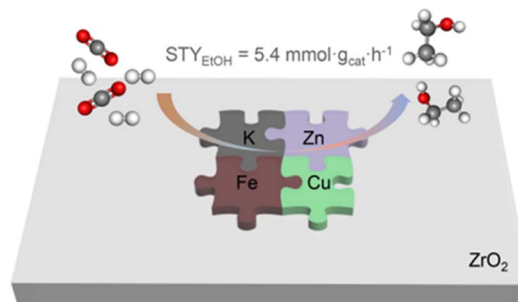
Sourav Gayen, Faneesha Assanar, Sampad Shyamal, Dorothy Priyanka Dorairaj and Sundargopal Ghosh\*



15925

### Ethanol synthesis *via* catalytic CO<sub>2</sub> hydrogenation over multi-elemental KFeCuZn/ZrO<sub>2</sub> catalyst

Pengfei Du, Abdellah Ait El Fakir,\* Shirun Zhao, Nazmul Hasan M. D. Dostagir, HongLi Pan, Kah Wei Ting, Shinya Mine, Yucheng Qian, Ken-ichi Shimizu\* and Takashi Toyao\*



## CORRECTION

15935

### Correction: Padlocking dihydrofurannulation for the control of small degree of helicity built on a fused-tetracyclic core

Arthur Gaucherand, Expédite Yen-Pon, Diego García-López, Jean-Valère Naubron, Sara Chentouf, Michel Giorgi, Stéphane Humbel, Marion Jean, Jean Rodriguez and Damien Bonne\*

