

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(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

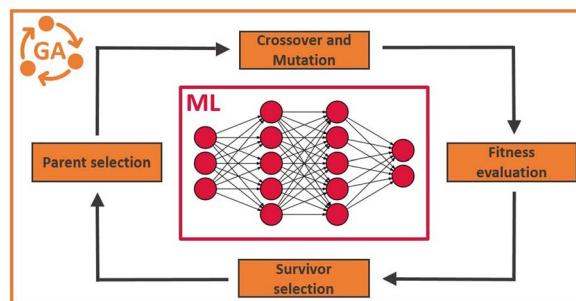
See Dean J. Tantillo *et al.*, pp. 15577–15587. Image reproduced by permission of Dean J. Tantillo from *Chem. Sci.*, 2024, 15, 15577.

PERSPECTIVE

15522

Augmenting genetic algorithms with machine learning for inverse molecular design

Hannes Kneiding and David Balcells*

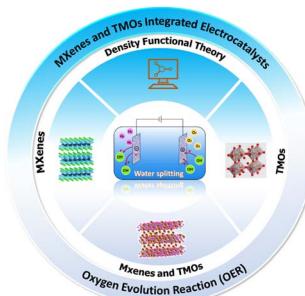


REVIEW

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 Arandiyan*



GOLD
OPEN
ACCESS

EES Solar

Exceptional research on solar
energy and photovoltaics

Part of the EES family

Join
in | Publish with us
rsc.li/EESSolar

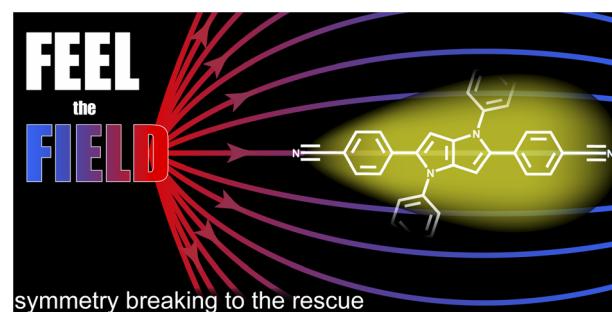


EDGE ARTICLES

15565

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

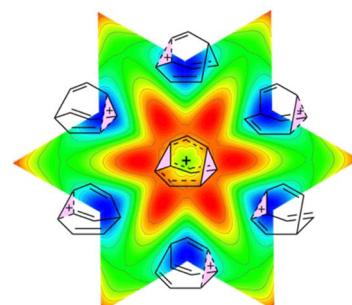
Bogdan Dereka,* Nikhil Maroli, Yevgen M. Poronik, Daniel T. Gryko and Alexei A. Kananenka



15577

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

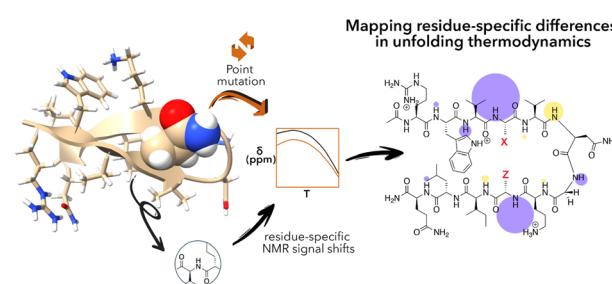
Wentao Guo, Wang-Yeuk Kong and Dean J. Tantillo*



15588

Probing the non-covalent forces key to the thermodynamics of β -hairpin unfolding

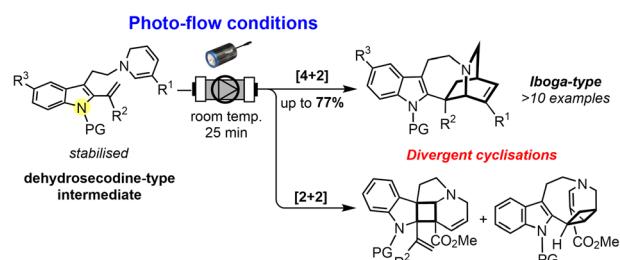
Thien H. Tran, Priyanka Prusty, Meghan Ricciardi, Christopher R. Travis, Marcey L. Waters and Bruce C. Gibb*



15599

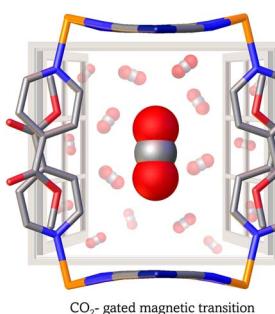
Direct photochemical intramolecular [4 + 2] cycloadditions of dehydrosecodine-type substrates for the synthesis of the iboga-type scaffold and divergent [2 + 2] cycloadditions employing micro-flow system

Gavin Tay, Soushi Nishimura and Hiroki Oguri*



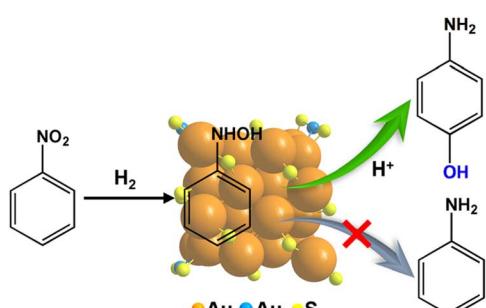
EDGE ARTICLES

15610

**CO₂-actuated spin transition tuning in an interdigitated Hofmann-type coordination polymer**

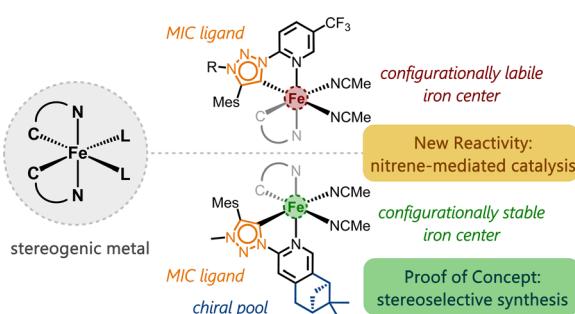
Abhik Paul, Wataru Kosaka, Bhart Kumar, Dibya Jyoti Mondal, Hitoshi Miyasaka* and Sanjit Konar*

15617

**Exclusive catalytic hydrogenation of nitrobenzene toward *p*-aminophenol over atomically precise Au₃₆(SR)₂₄ clusters**

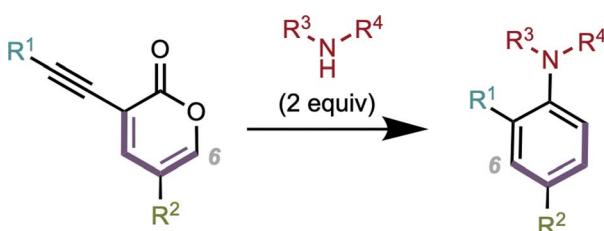
Jinzhi Lu, Kun Tang, Guodong Qi, Chao Juan, Jun Xu, Zhenfeng Cai, Dan Li,* Xiao Cai, Xu Liu, Mingyang Chen,* Weiping Ding and Yan Zhu*

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

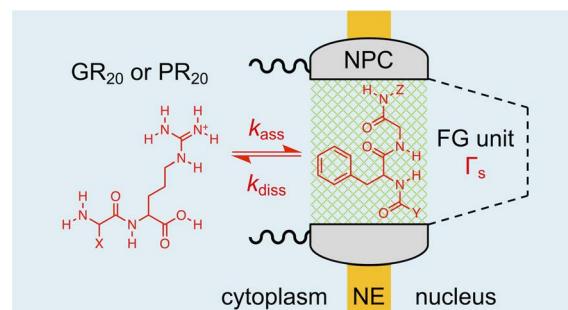


EDGE ARTICLES

15639

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

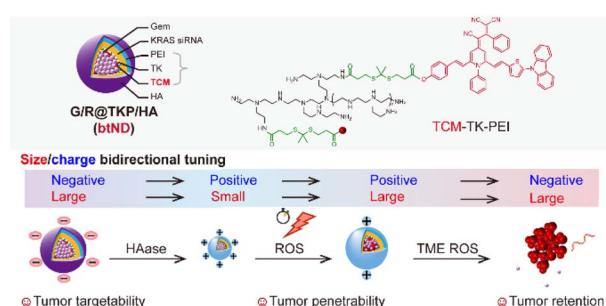
Siao-Han Huang, Moghitha Parandhaman, Manu Jyothi Ravi, Donald C. Janda and Shigeru Amemiya*



15647

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

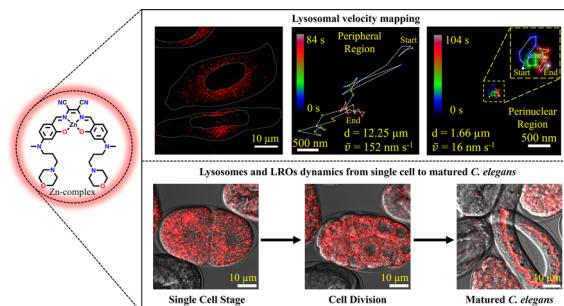
Yiqi Shi, Jinghan Liao, Cuiyun Zhang, Qi Wu, Shanshan Hu, Ting Yang, Jihong Liu, Zhirong Zhu, Wei-Hong Zhu and Qi Wang*



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

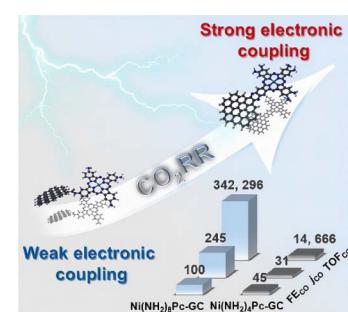
Abdul Salam, Kush Kaushik, Bodhidipra Mukherjee, Farhan Anjum, Goraksha T. Sapkal, Shagun Sharma, Richa Garg and Chayan Kanti Nandi*



15670

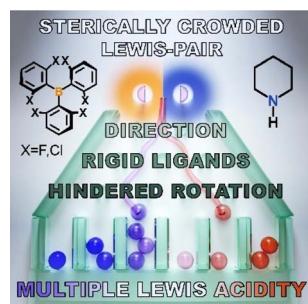
Graphite conjugated nickel phthalocyanine for efficient CO₂ electroreduction and Zn–CO₂ batteries

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



EDGE ARTICLES

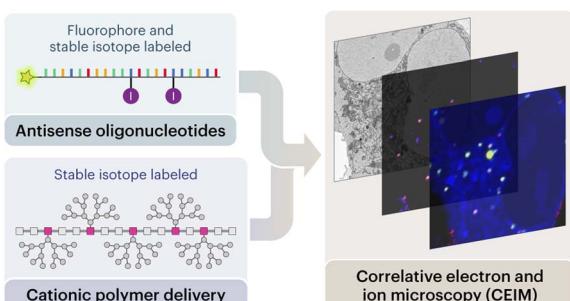
15679



Illuminating the multiple Lewis acidity of triarylboranes via atropisomeric dative adducts

Benj  m  n Kov  cs, Tam  s F  ld  s, M  rk Szab  ,   va Dork  , Bianka K  tai, Gergely Laczk  , Tam  s Holczbauer, Attila Domj  n,* Imre P  p  i* and Tibor So  s*

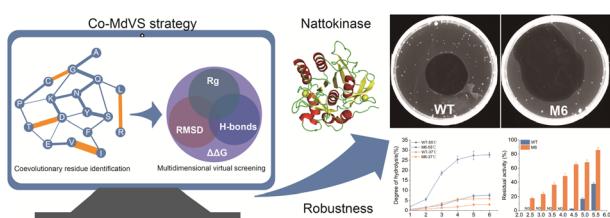
15690



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, Qiongxian Lin, Udit Bhatt, Stephen G. Young, Nicole M. Smith, Mehran Nikan, Clive A. Prestidge, Haibo Jiang* and K. Swaminathan Iyer*

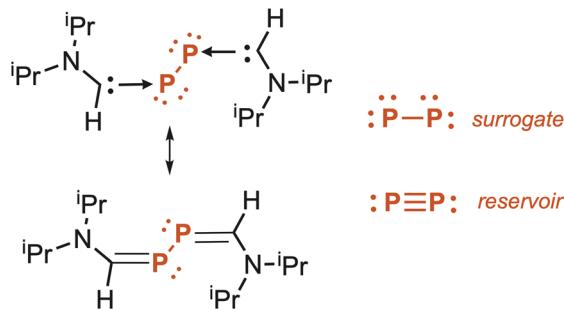
15698



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*

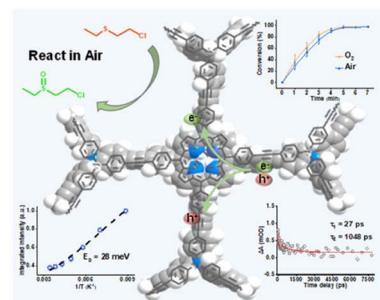


EDGE ARTICLES

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

N₂H₄Zn(HC₃N₃O₃): exceptionally strong second harmonic generation and ultra-long phosphorescence

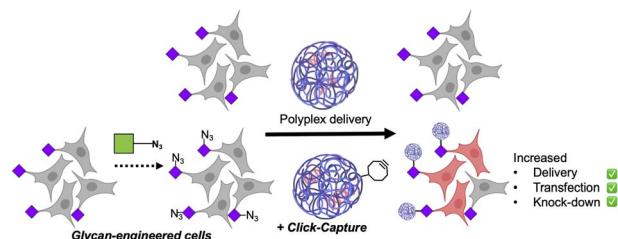
Can Yang, Yuwei Kang, Xuefei Wang, Jie Gou, Yi Xiong, Zece Zhu, Ling Chen* and Qi Wu*



15731

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

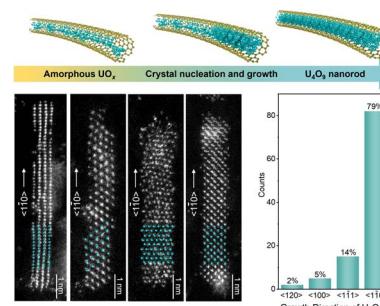
Qiao Tang, Ruben M. F. Tomás and Matthew I. Gibson*



15737

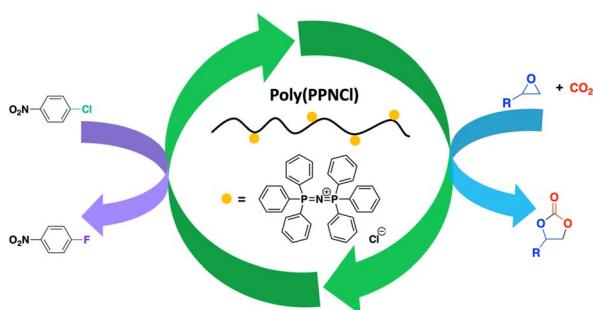
Directional growth and reconstruction of ultrafine uranium oxide nanorods within single-walled carbon nanotubes

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



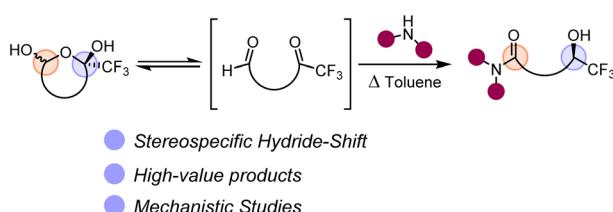
EDGE ARTICLES

15745

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

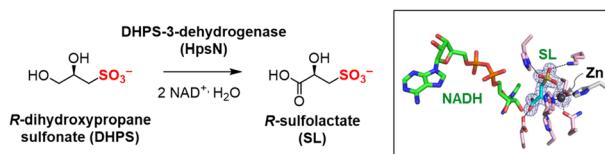
Ziwei Xu, Meng Wang and Michael P. Shaver*

15751

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

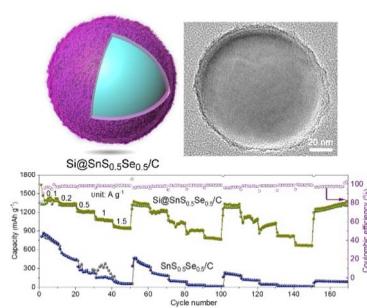
Roberto Tinelli, Manuel Schupp, Immo Klose, Saad Shaaban, Boris Maryasin, Leticia González and Nuno Maulide*

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_{0.5}Se_{0.5}/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*

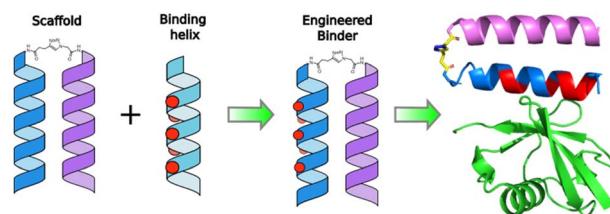


EDGE ARTICLES

15776

An engineered ubiquitin binding coiled coil peptide

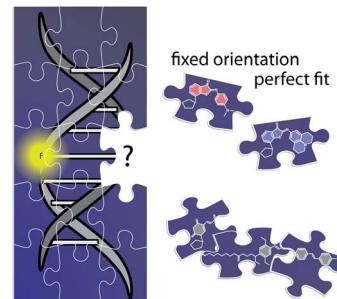
Pernille Vosbein, Paula Paredes Vergara, Danny T. Huang and Andrew R. Thomson*



15783

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

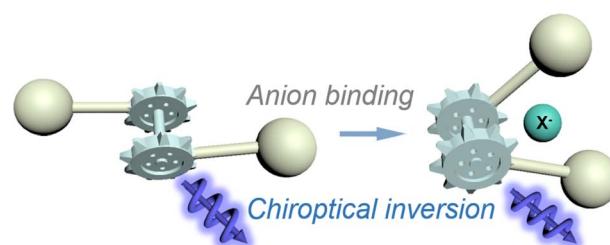
Larita Luma, Judith C. Pursteiner, Tobias Fischer, Rainer Hegger, Irene Burghardt,* Josef Wachtveitl* and Alexander Heckel*



15790

A photoactivated chiral molecular clamp rotated by selective anion binding

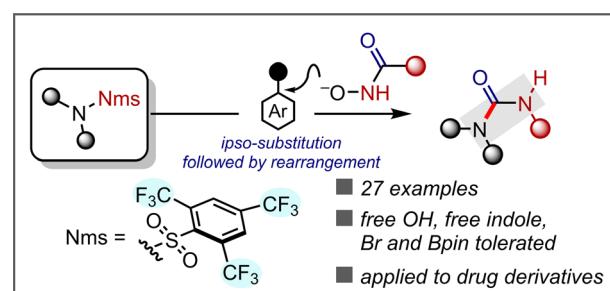
Yiping Liu, Aiyou Hao and Pengyao Xing*



15799

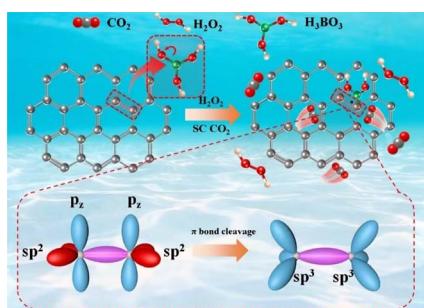
Deprotective Lossen rearrangement: a direct and general transformation of Nms-amides to unsymmetrical ureas

Philipp Spieß, Jakub Brześkiewicz and Nuno Maulide*



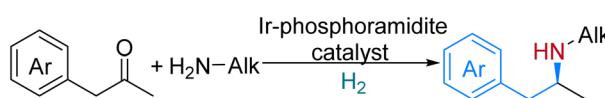
EDGE ARTICLES

15804

**Introduction of the $-B(OH)_2$ group into a graphene motif for p_z orbital removal and ferromagnetic modulation**

Di Zhang, Bo Gao, Yuqi Ouyang, Song Xu,* Qingyong Tian, Wenzhuo Wu and Qun Xu*

15811

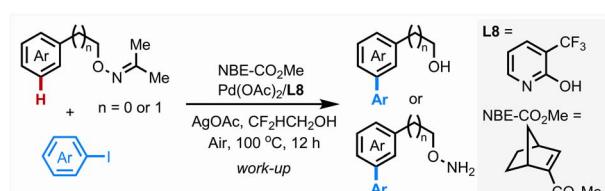


- ★ Low cata. loading (0.03 mol%) ★ Additive-free conditions
- ★ Broad ketone substrate scope ★ Alkylamine sources
- ★ Ligands with 3 blocking planes ★ Multiple drug synthesis

Direct synthesis of chiral β -arylamines via additive-free asymmetric reductive amination enabled by tunable bulky phosphoramidite ligands

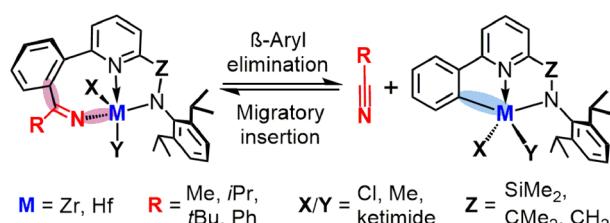
Jing Wang, Wenji Wang, Haizhou Huang, Zhiqing Ma and Mingxin Chang*

15819

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

Hua-Chen Shen, Jian-Jun Li, Peng Wang* and Jin-Quan Yu*

15825

**Reversible C–C bond formation in group 4 metal complexes: nitrile extrusion via β -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*

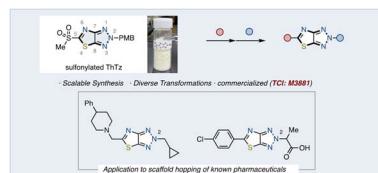


EDGE ARTICLES

15835

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

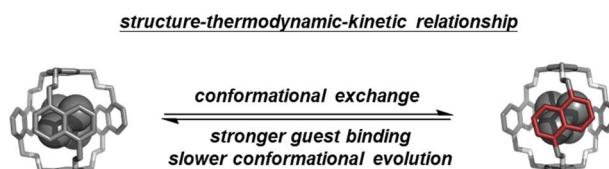
Ryuya Miyazaki, Fumito Takada, Takunari Kikuchi, Yuya Oguro, Makoto Kamata, Takafumi Yukawa, Kenta Kato, Kei Muto* and Junichiro Yamaguchi*



15841

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

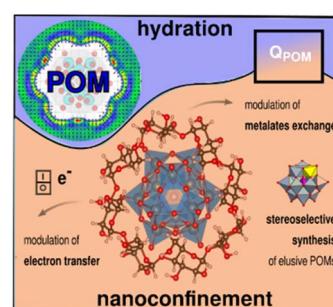
Shan He, Mao Quan, Liu-Pan Yang, Ho Yu Au-Yeung* and Wei Jiang



15849

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

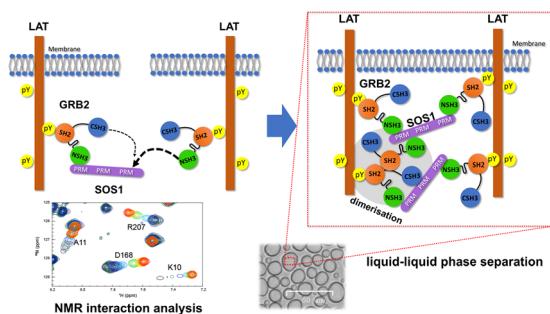
Mireia Segado-Centellas,* Clément Falaise,* Nathalie Leclerc, Gabrielle Mpakko Priso, Mohamed Haouas, Emmanuel Cadot and Carles Bo



15858

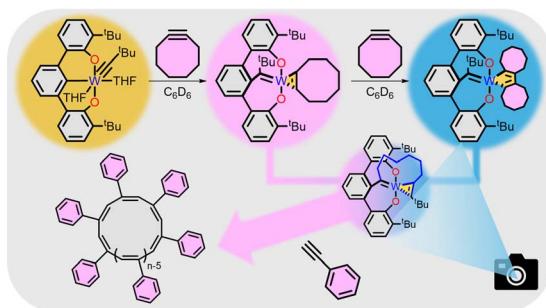
Different molecular recognition by three domains of the full-length GRB2 to SOS1 proline-rich motifs and EGFR phosphorylated sites

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



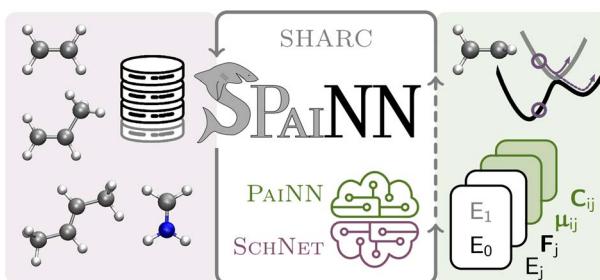
EDGE ARTICLES

15873

**Snapshot of cyclooctyne ring-opening to a tethered alkylidene cyclic polymer catalyst**

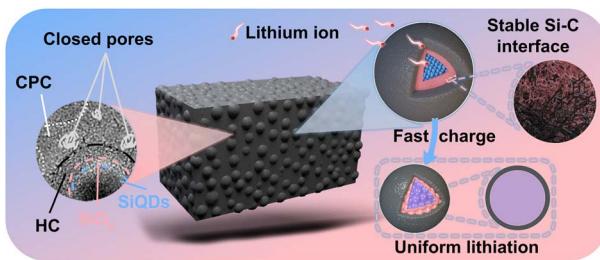
Javier M. Hurst, Rinku Yadav, Parker T. Boeck, Ion Ghiviriga, ChristiAnna L. Brantley, Łukasz Dobrzański and Adam S. Veige*

15880

**SPAIINN: equivariant message passing for excited-state nonadiabatic molecular dynamics**

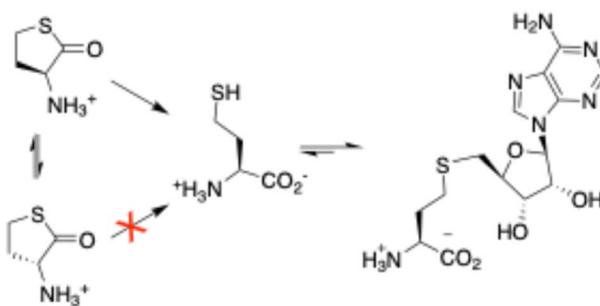
Sascha Mausenberger, Carolin Müller,* Alexandre Tkatchenko, Philipp Marquetand, Leticia González and Julia Westermayr*

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*

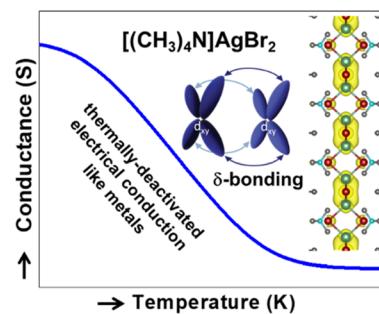


EDGE ARTICLES

15907

Ultralow thermal conductivity and thermally-deactivated electrical transport in a 1D silver array with alternating δ -bonds

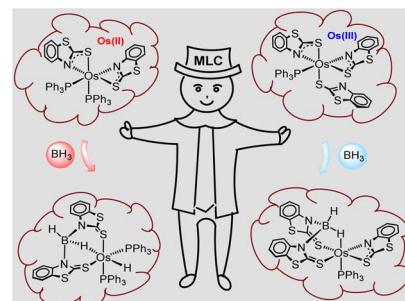
Nahid Hassan, Suneetha Nagaraja, Sauvik Saha, Kartick Tarafder and Nirmalya Ballav*



15913

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

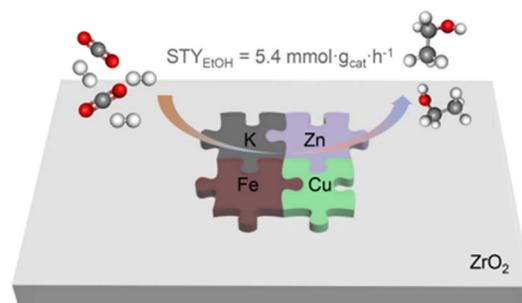
Sourav Gayen, Faneesha Assanar, Sampad Shyamal, Dorothy Priyanka Dorairaj and Sundargopal Ghosh*



15925

Ethanol synthesis via catalytic CO₂ hydrogenation over multi-elemental KFeCuZn/ZrO₂ 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 dihydrofuran annulation 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*

