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IN THIS ISSUE

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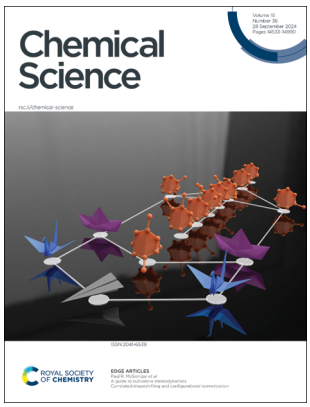


Cover
See Paul McGonigal *et al.*, pp. 14608–14617 and 14618–14624. Image reproduced by permission of Paul McGonigal from *Chem. Sci.*, 2024, **15**, 14608 and 14618.

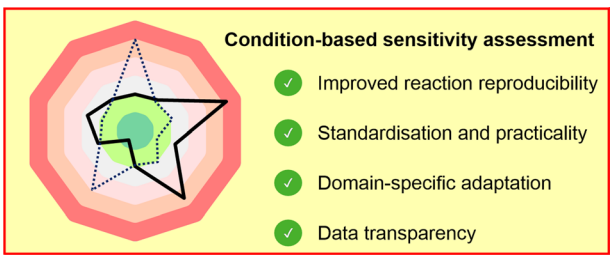
Inside cover
See Shusuke Tomoshige, Minoru Ishikawa *et al.*, pp. 14625–14634. Image reproduced by permission of Shusuke Tomoshige from *Chem. Sci.*, 2024, **15**, 14625.

PERSPECTIVE

14548

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

Felix Schäfer, Lukas Lückemeier and Frank Glorius*

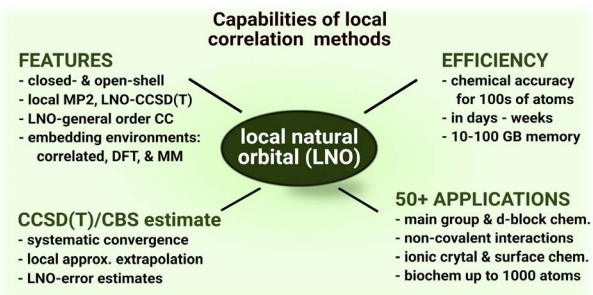


REVIEWS

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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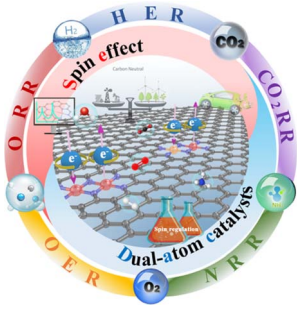
REVIEWS

14585

Spin effect in dual-atom catalysts for electrocatalysis

Xiaoqin Xu and Jingqi Guan*

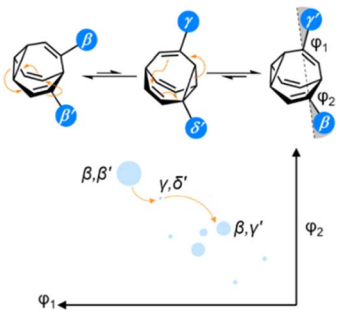


EDGE ARTICLES

14608

A guide to bullvalene stereodynamics

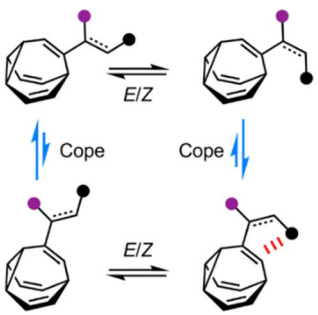
Robert A. Ives, William Maturi, Matthew T. Gill, Conor Rankine* and Paul R. McGonigal*



14618

Correlated shapeshifting and configurational isomerization

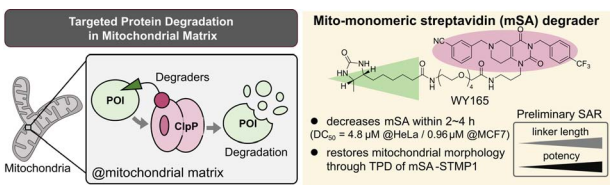
Burhan A. Hussein, William Maturi, Mary Kate Rylands, Aisha N. Bismillah, Yuzhen Wen, Juan A. Aguilar, Rabia Ayub, Conor D. Rankine and Paul R. McGonigal*



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*



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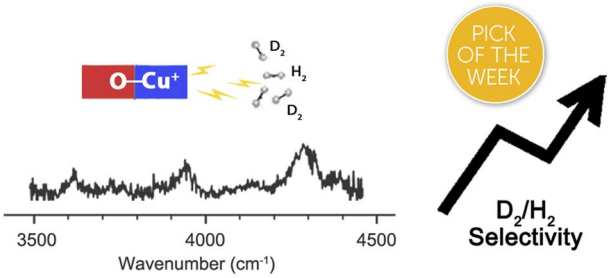
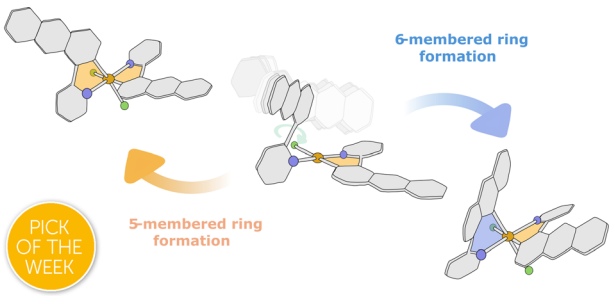


Direct evidence for ligand-enhanced activity of Cu(I) sites

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

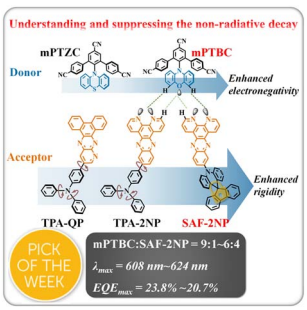
14644



π-Extended ligands with dual-binding behavior: hindered rotation unlocks unexpected reactivity in cyclometalated Pt complexes

Seiya Ota, Miguel A. Soto,* Brian O. Patrick, Saeid Kamal, Francesco Lelj and Mark J. MacLachlan*

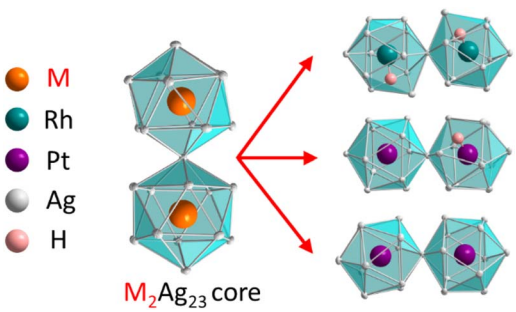
14651



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,* Yong-Hao Zheng, Hui Wang, Hui Lin, Si-Lu Tao, Cai-Jun Zheng* and Xiao-Hong Zhang*

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*

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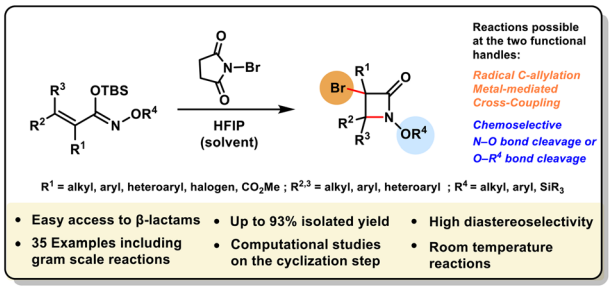
EDGE ARTICLES

14668

Forging structural complexity: diastereoselective synthesis of densely substituted β-lactams with dual functional handles for enhanced core modifications

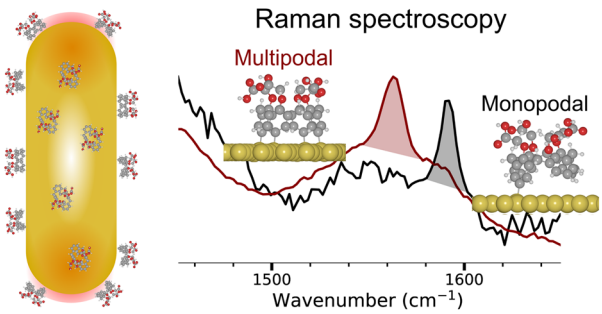
Agustin M. Rodriguez Treviño, Pierre Loch-Temzelides, Sanjay Pandiri, Justin K. Kirkland, Michael T. Davenport, Ulises Aguinaga, Muhammed Yousufuddin, Daniel H. Ess and László Kürti*



14677

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

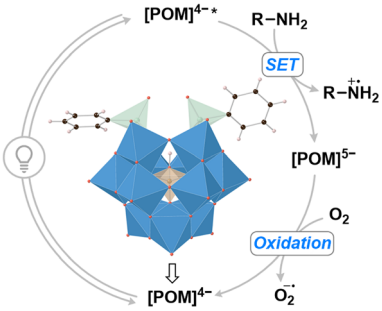
Auguste Tetenoire, Anna Omelchuk, Volodymyr Malytskyi, Ivan Jabin, Victor Lepeintre, Gilles Bruylants, Yun Luo, Arnaud Fihey, Mikaël Kepenekian* and Corinne Lagrost*



14685

Organofunctionalized borotungstate polyoxometalates as tunable photocatalysts for oxidative dimerization of amines

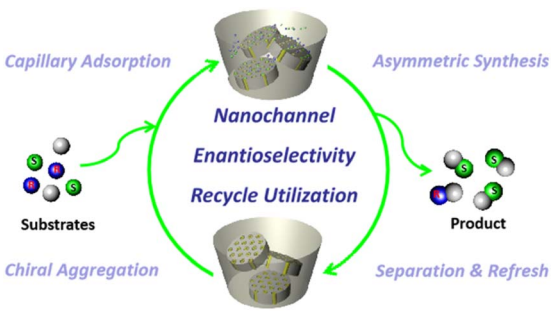
Nicole Tsang, Alexander J. Kibler, Stephen P. Argent, Hon Wai Lam,* Kieran D. Jones* and Graham N. Newton*



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*



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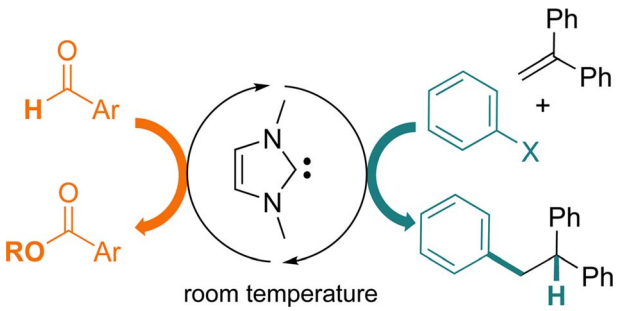
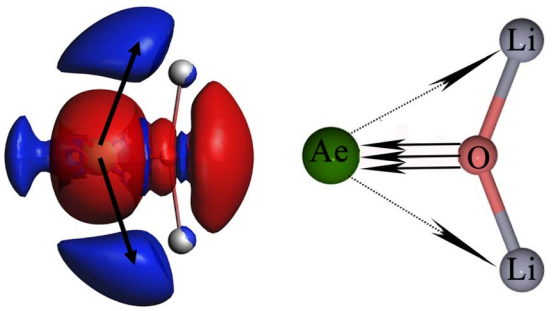


A simple N-heterocyclic carbene for the catalytic up-conversion of aldehydes into stoichiometric super electron donors

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

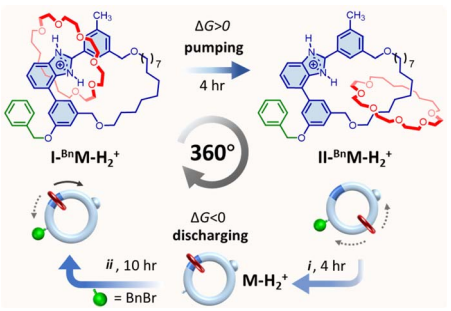
14705



Unusual quadruple bonds featuring collective interaction-type σ 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*

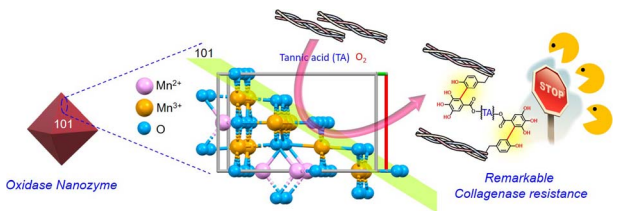
14721



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*

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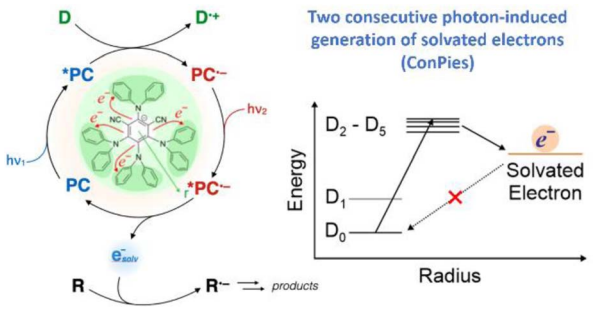
14739

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

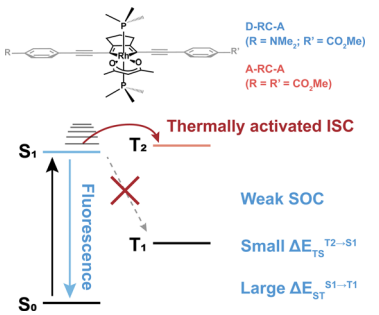
Marco Villa, Andrea Fermi, Francesco Calogero, Xia Wu, Andrea Gualandi, Pier Giorgio Cozzi, Alessandro Troisi,* Barbara Ventura* and Paola Ceroni*



14746

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

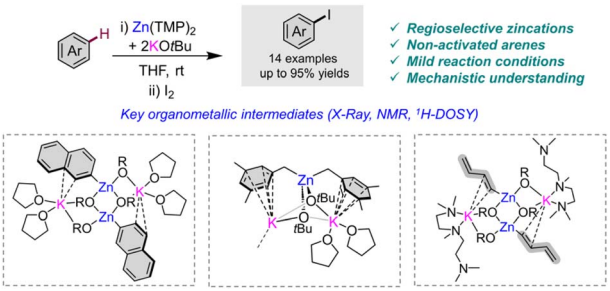
Zilong Guo, Yaxin Wang, Julia Heitmüller, Carolin Sieck, Andreas Prüfer, Philipp Ralle, Andreas Steffen, Petr Henke, Peter R. Ogilby,* Todd B. Marder,* Xiaonan Ma* and Tobias Brixner*



14757

Combining two relatively weak bases ($Zn(TMP)_2$ and KO*t*Bu) for the regioselective metalation of non-activated arenes and heteroarenes

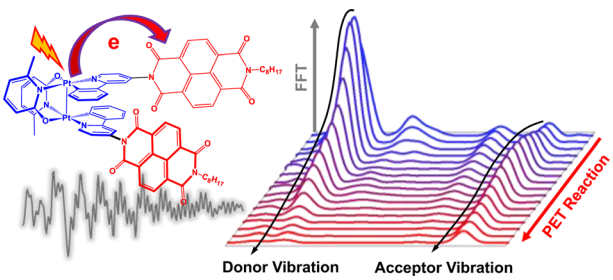
Neil R. Judge and Eva Hevia*



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*



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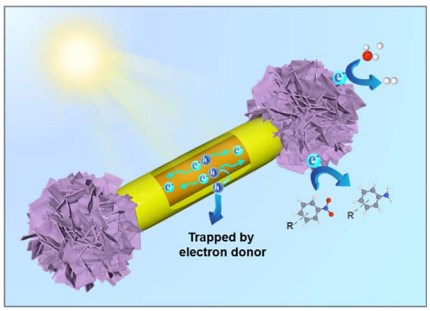
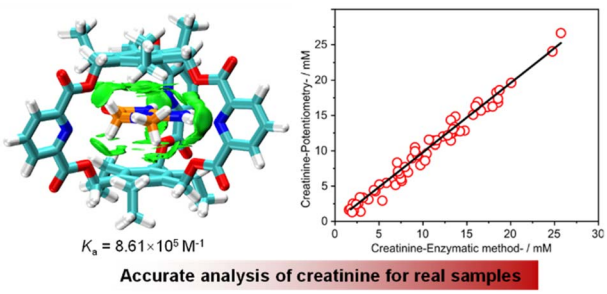


Customizing dumbbell-shaped heterostructured artificial photosystems steering versatile photoredox catalysis

Peng Su, Xian Yan and Fang-Xing Xiao*

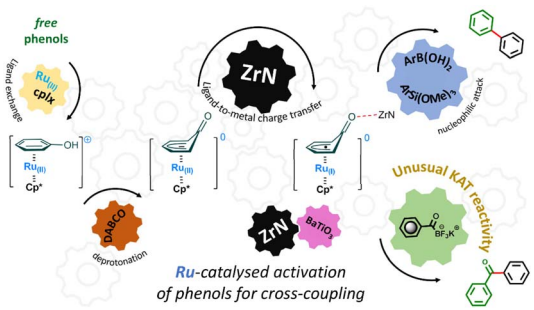
14791



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*

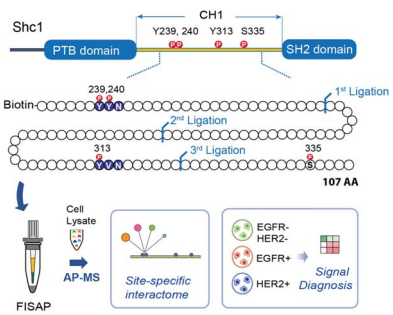
14798



Ru-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*

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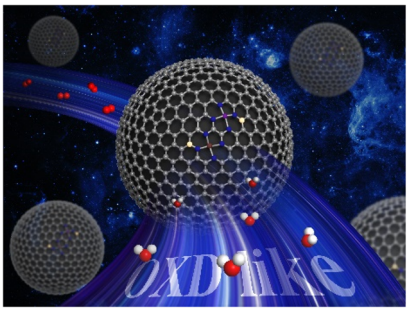
14816

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

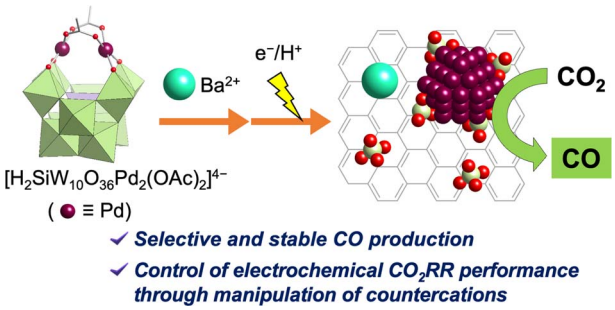
Huan Cheng, Yanyue Chen, Mingjia Liu, Hongling Tao, Lu Chen, Fupeng Wang, Long Huang, Jian Tang,* Tong Yang* and Rong Hu*



14829

Pd-incorporated polyoxometalate catalysts for electrochemical CO_2 reduction

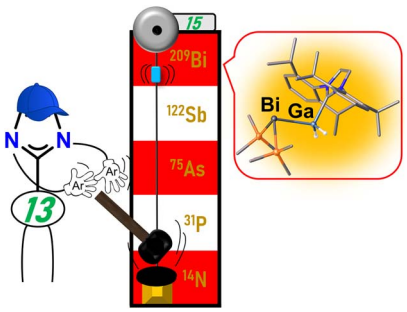
Kimitake Kawakami, Tomohiro Yabe, Fumiaki Amano, Kazuya Yamaguchi and Kosuke Suzuki*



14837

Synthesis of bismuthanyl-substituted monomeric triel hydrides

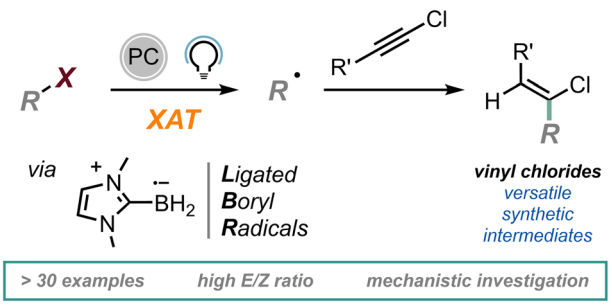
Robert Szlosek, Christian Marquardt, Oliver Hegen, Gábor Balázs, Christoph Riesinger, Alexey Y. Timoshkin and Manfred Scheer*



14844

Visible light-induced halogen-atom transfer by N-heterocyclic carbene-ligated boryl radicals for diastereoselective C(sp^3)–C(sp^2) bond formation

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



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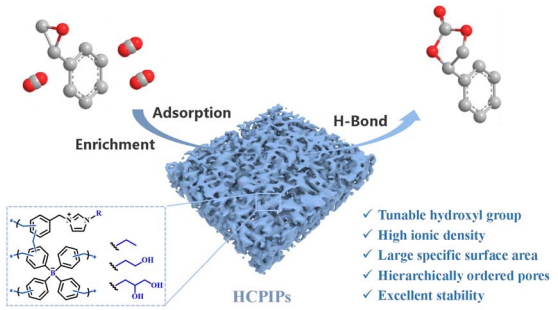
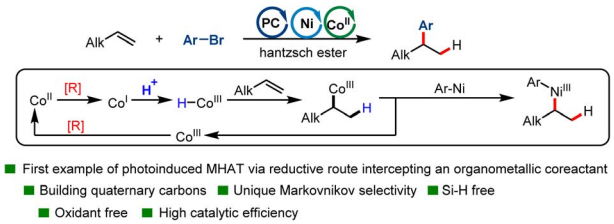
14851



Non-cationic hyper-crosslinked ionic polymers with hierarchically ordered porous structures: facile synthesis and applications for highly efficient CO_2 capture and conversion

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

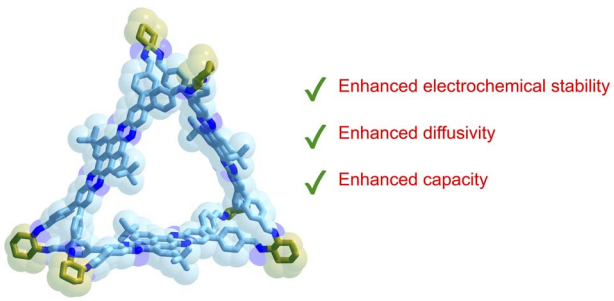
14865



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*

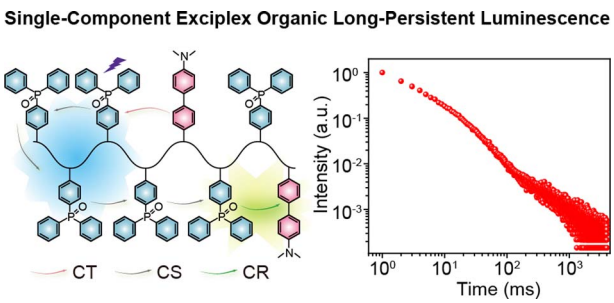
14872



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



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*

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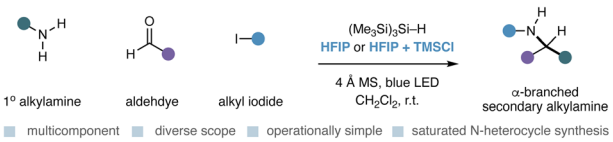
EDGE ARTICLES

14888

Modular synthesis of α-branched secondary alkylamines *via* visible-light-mediated carbonyl alkylative amination

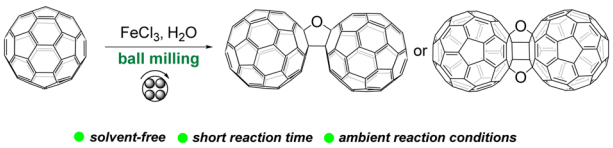
Milo A. Smith, Ryan J. D. Kang, Roopender Kumar, Biswarup Roy and Matthew J. Gaunt*



14899

Unexpected and divergent mechanosynthesis of furanoid-bridged fullerene dimers $C_{120}O$ and $C_{120}O_2$

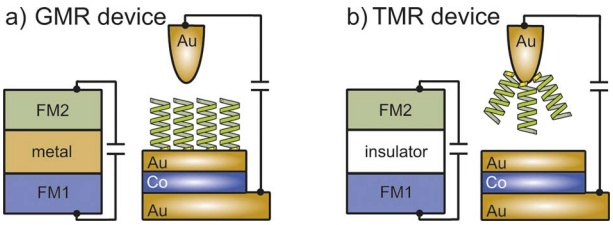
Gang Shao, Yuan-Yuan Liu, Chuang Niu, Zheng-Chun Yin, Shi-Qi Ye, Yang-Rong Yao, Muqing Chen, Jun-Shen Chen, Xu-Ling Xia, Shangfeng Yang* and Guan-Wu Wang*



14905

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

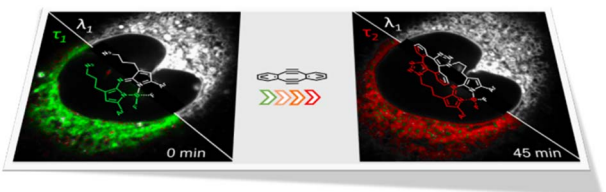
Thi Ngoc Ha Nguyen, Georgeta Salvan, Olav Hellwig, Yossi Paltiel, Lech Thomasz Baczewski and Christoph Tegenkamp*



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*



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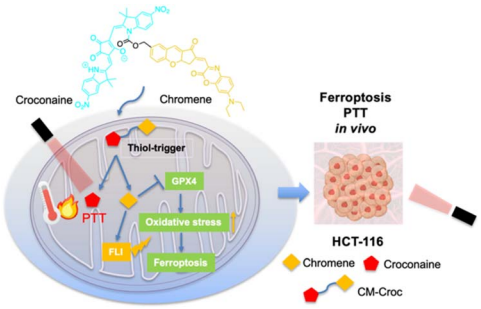
EDGE ARTICLES

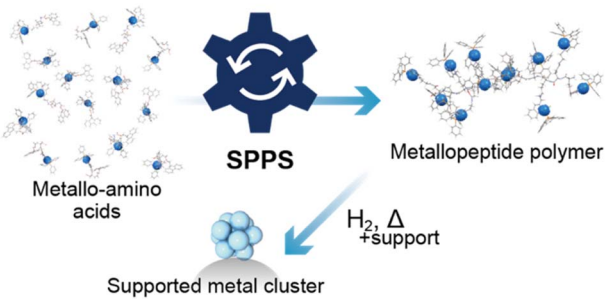
14924



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*

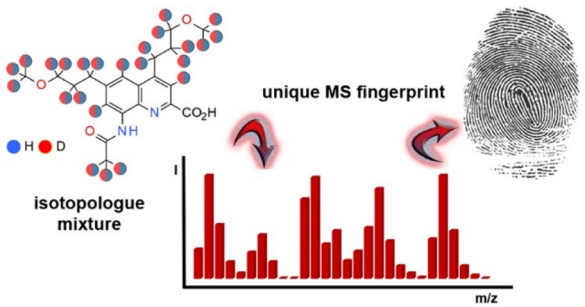
14931



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, Miftakhul Huda, Makoto Tanabe, Wang-Jae Chun and Kimihisa Yamamoto*

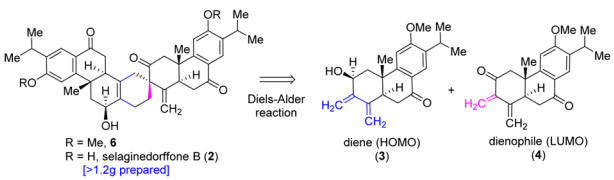
14938



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, Debgopal Jana, Nilangshu Mandal, Ayan Mondal, Ranjit Murmu, Nanda Kishore Roy, Ayan Datta* and Alakesh Bisai*

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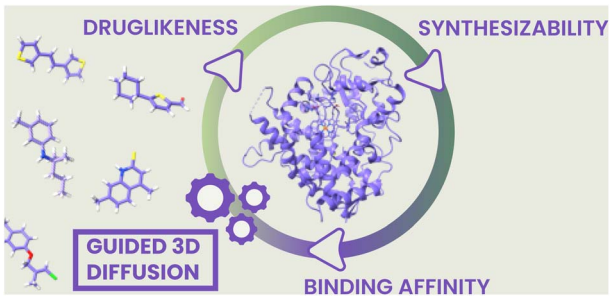
EDGE ARTICLES

14954

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

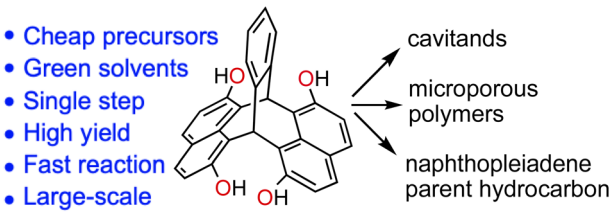
Julian Cremer,* Tuan Le,* Frank Noé, Djork-Arné Clevert and Kristof T. Schütt



14968

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

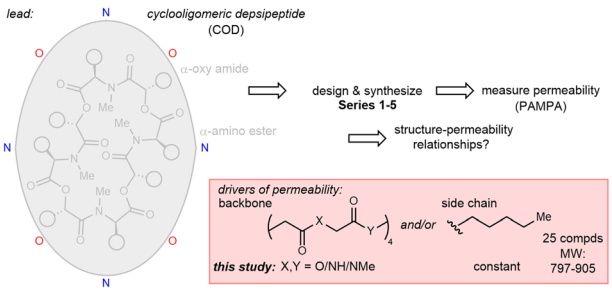
Md Khairul Amin, Chunchun Ye, Shuhua Pang, Yuancheng Liu, Dominic Taylor, Gary S. Nichol and Neil B. McKeown*



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 Otoya, Kane T. McQuaid, Neil G. Paterson, David J. Cardin, Andrew Kellett and Christine J. Cardin*