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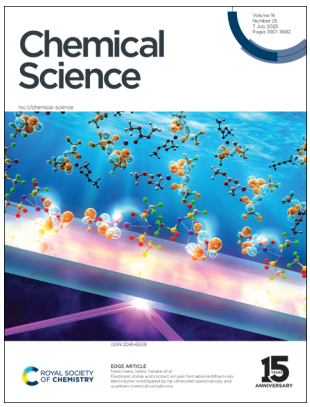
IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 16(25) 11167–11682 (2025)



Cover
See Nami Ueno, Ichiro Tanabe *et al.*, pp. 11232–11239. Image reproduced by permission of Ichiro Tanabe from *Chem. Sci.*, 2025, **16**, 11232.

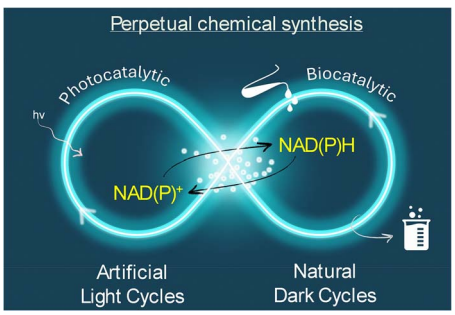
Inside cover
See Kanta Kawai, Tasuku Hirayama *et al.*, pp. 11240–11245. Image reproduced by permission of Kanta Kawai from *Chem. Sci.*, 2025, **16**, 11240.

PERSPECTIVE

11184

A path to perpetual chemical synthesis *via* photocatalytic cofactor regeneration

Vanshika Jain* and Pramod P. Pillai*

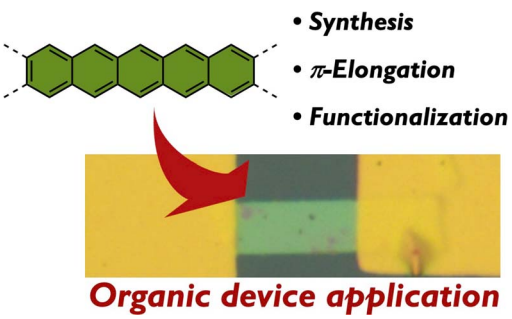


REVIEW

11204

Exploring the chemistry of higher acenes: from synthesis to applications

Hironobu Hayashi* and Hiroko Yamada*



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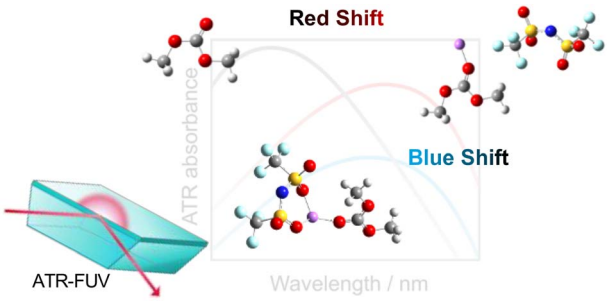
EDGE ARTICLES

11232

Electronic states and contact ion pair formation in lithium-ion electrolytes investigated by far-ultraviolet spectroscopy and quantum chemical calculations

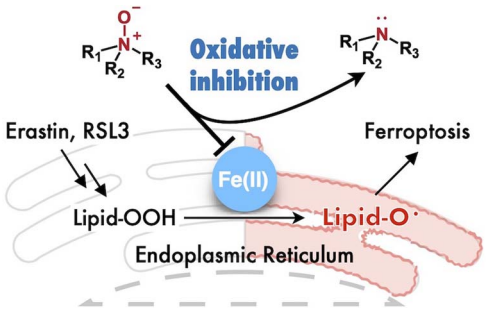
Hitomi Sato, Nami Ueno* and Ichiro Tanabe*



11240

Inhibition of ferroptosis by *N*-oxide-based fluorescent probes *via* selective oxidation of ferrous ions

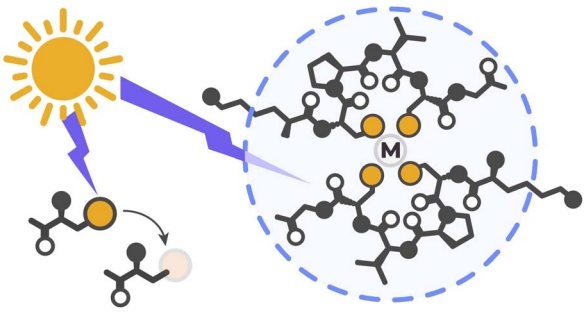
Kanta Kawai, Rie Haruki, Shunsuke Nozawa, Hideko Nagasawa and Tasuku Hirayama*



11246

Preferential survival of prebiotic metallopeptides in the presence of ultraviolet light

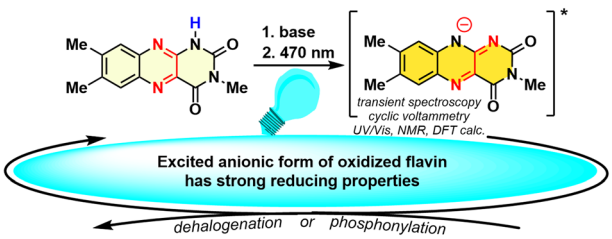
Daniele Rossetto, Serge Nader, Corinna L. Kufner, Gabriella G. Lozano, Linda Cerofolini, Marco Fragai, Vlad Martin-Diaconescu, Barbara Zambelli, Stefano Ciurli, Graziano Guella, Rafał Szabla, Dimitar D. Sasselov and Sheref S. Mansy*



11255

Introduction of flavin anions into photoredox catalysis: acid–base equilibria of lumichrome allow photoreductions with an anion of an elusive 10-unsubstituted isoalloxazine

Dorota Prukała,* Ekaterina Zubova, Eva Svobodová, Ludmila Šimková, Naisargi Varma, Josef Chudoba, Jiří Ludvík, Gotard Burdzinski, Iwona Gulaczyk, Marek Sikorski* and Radek Cibulka*



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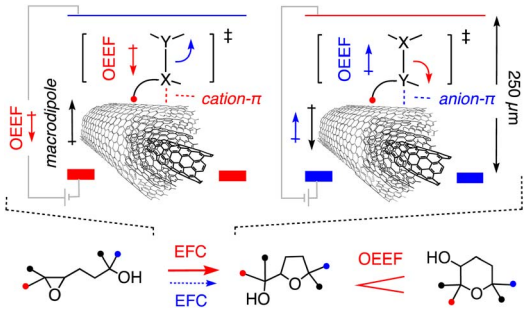
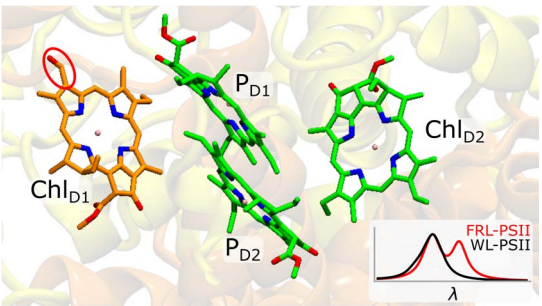


Response of reaction mechanisms to electric-field catalysis on carbon nanotubes in microfluidic reactors

M. Ángeles Gutiérrez López, Alenka Marsalek, Naomi Sakai and Stefan Matile*

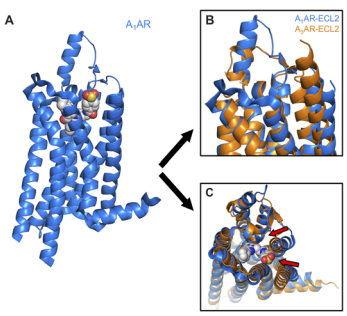
11270



Modified chlorophyll pigment at Chl_{D1} tunes photosystem II beyond the red-light limit

Friederike Allgöwer, Abhishek Sirohiwal, Ana P. Gamiz-Hernandez, Maximilian C. Pöverlein, Andrea Fantuzzi, A. William Rutherford and Ville R. I. Kaila*

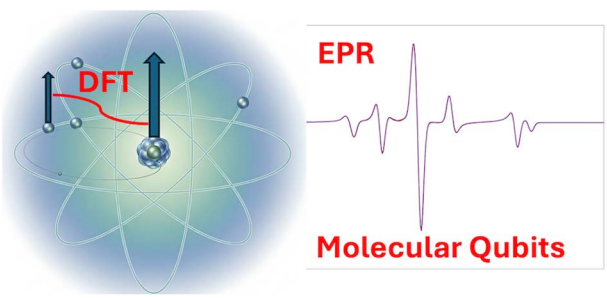
11280



Enhancing binding affinity predictions through efficient sampling with a re-engineered BAR method: a test on GPCR targets

Minkyu Kim, Jian Jeong, Donghwan Kim, Sangbae Lee* and Art E. Cho*

11291



Exploring hyperfine coupling in molecular qubits

Joan Cardona, Àlex Solé, Pablo Mella, Daniel Aravena,* Javier Ruiz-Hidalgo,* Silvia Gómez-Coca* and Eliseo Ruiz*

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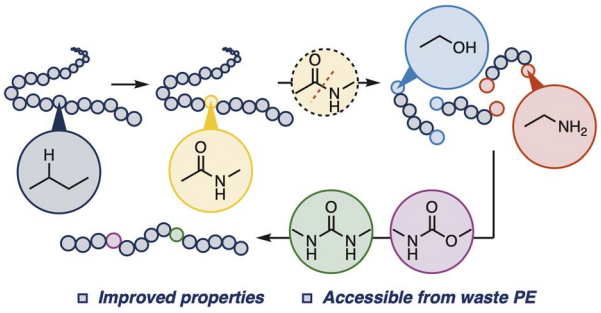
EDGE ARTICLES

11304

Backbone editing and deconstruction of polyethylene by Beckmann rearrangement and hydrogenolysis

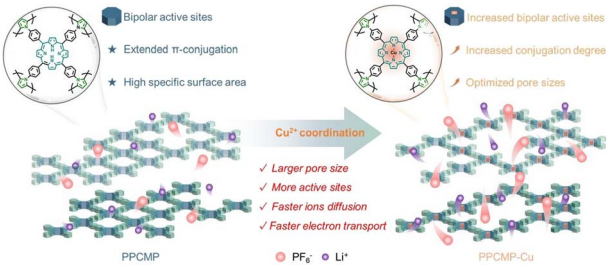
Jake X. Shi, Diane D. Kim, Nicodemo R. Ciccia, Pierre Lahaie-Boivin and John F. Hartwig*



11311

Cu-mediated bipolar-type extended π-conjugated microporous polymers for lithium-ion battery cathodes with high energy density and fast-charging capability

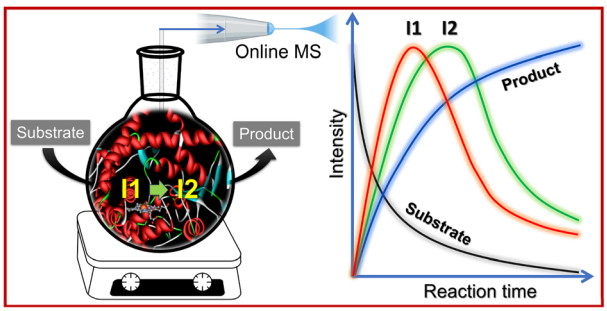
Yitao Li, Ju Duan, Yuzhu Wang, Likuan Teng, He Liu, Jiaqiang Li, Mengqi Liu, Weisi He, Huawei Hu, Lulu Wang, Wei Lyu* and Yaozu Liao*



11322

Real-time capture of reactive intermediates in an enzymatic reaction: insights into a P450-catalyzed oxidation

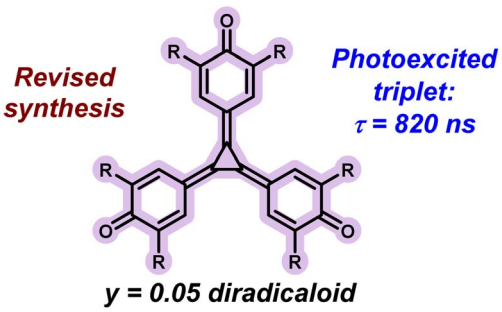
Pragya Pahchan, Abhijit Nandy, Eswarayya Ramireddy* and Shibdas Banerjee*



11331

Photoexcited and ground-state diradical(oid) character in a triquino[3]radialene

Bethany K. Hillier, Damon M. de Clercq, Stephen D. S. Bortolussi, Simona S. Capomolla, Michael P. Nielsen, Katarzyna Młodzikowska-Pieńko, Renana Gershoni-Poranne, Timothy W. Schmidt and Martin D. Peeks*



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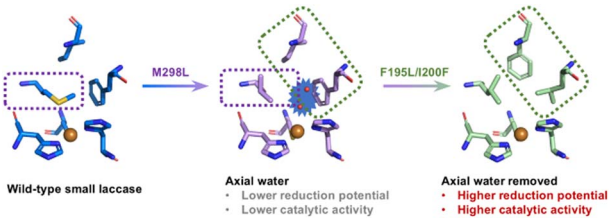
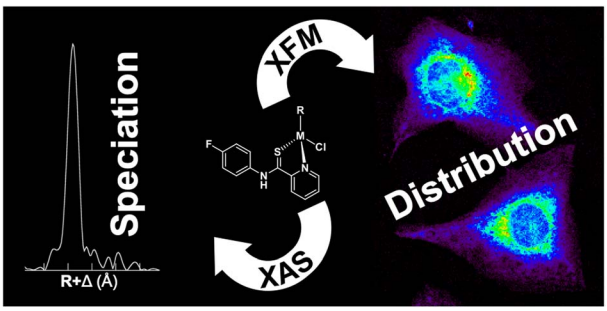


Unexpected effect of an axial ligand mutation in the type 1 copper center in small laccase: structure-based analyses and engineering to increase reduction potential and activity

Jing-Xiang Wang, Avery C. Vilbert, Lucas H. Williams, Evan N. Mirts, Chang Cui and Yi Lu*

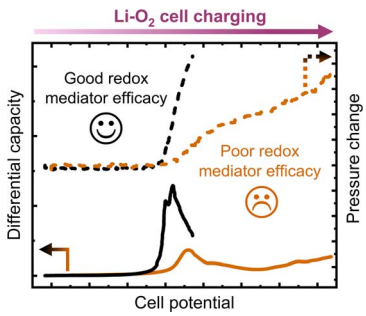
11347



X-ray fluorescence microscopy and X-ray absorption spectroscopy reveal the stability of the plecstatin-1 scaffold in biological model systems: comparison of Ru, Os and Ir analogues

James H. Lovett, Barry P. Lai, Hugh O. Bloomfield, Ani T. Baker, Matthew P. Sullivan, Christian G. Hartinger and Hugh H. Harris*

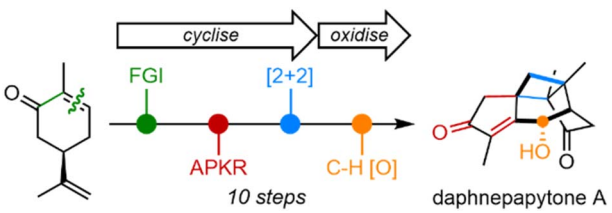
11359



Multicycle *operando* pressure measurements enable assessment of redox mediator efficacy in lithium–oxygen batteries

Thukshan Samarakoon, Ben Wood, Alex R. Neale, Elliot Coulbeck, Daniel J. Saccomando and Laurence J. Hardwick*

11375



Bio-inspired total synthesis of daphnepapytone A

Joan Pereira, Nicolas Casaretto, Gilles Frison and Bastien Nay*

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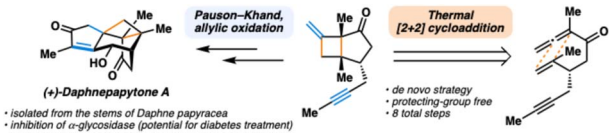
11381

Concise total synthesis of the cage-like sesquiterpenoid (+)-daphnepapytone A

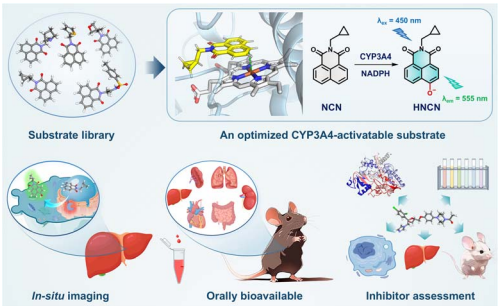
Elijah C. Gonzalez, Isabel M. de la Torre Roehl and Brian M. Stoltz*



11386

An optimized CYP3A4-activatable fluorogenic sensor for *in situ* functional imaging and multi-dimensional inhibitor assessment

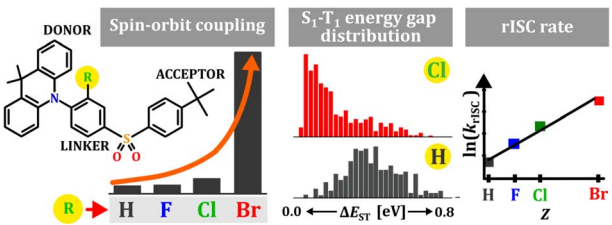
Feng Zhang, Yufan Fan, Mei Luo, Jian Huang, Bei Zhao, Lin Chen, Guanghao Zhu, Yuan Xiong, Hong Lin, Chuting Xu, Xiaodi Yang, Tony D. James* and Guangbo Ge*



11398

Pursuing the holy grail of thermally activated delayed fluorescence emitters: a molecular strategy for reducing the energy gap and enhancing spin–orbit coupling

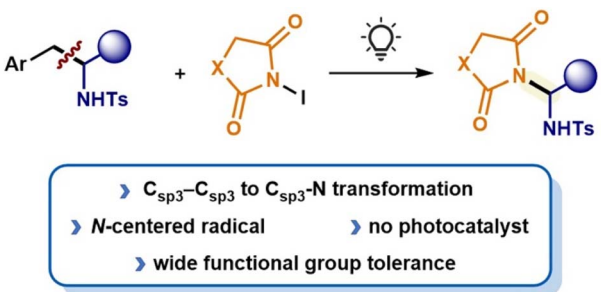
Vladyslav Ievtukhov, Antonio Prlj, Olga Ciupak, Michał Mońka and Illia E. Serdiuk*



11413

Visible-light-initiated metal-free C_{sp^3}–C_{sp^3} to C_{sp^3}–N conversion in homobenzylic sulfonamides with *N*-iodoimides

Guillermo Morales-Ortega, Estíbaliz Merino and Javier Carreras*



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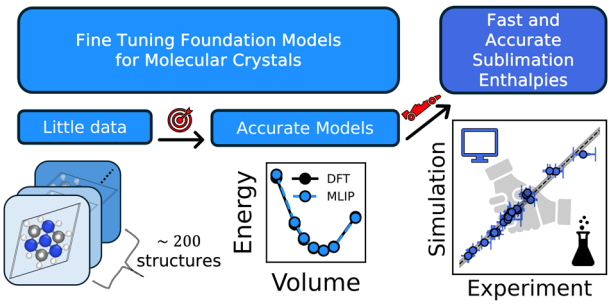
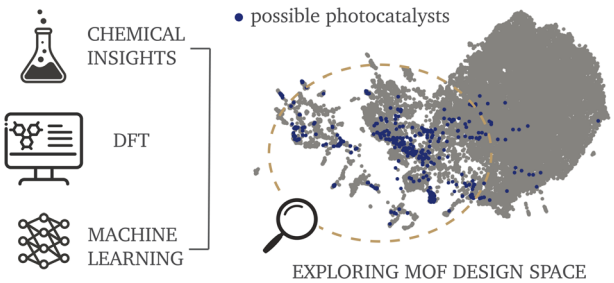


Accurate and efficient machine learning interatomic potentials for finite temperature modelling of molecular crystals

Flaviano Della Pia, Benjamin X. Shi, Venkat Kapil, Andrea Zen, Dario Alfè and Angelos Michaelides*

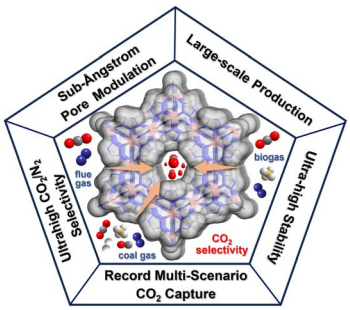
11434



Exploring the chemical design space of metal–organic frameworks for photocatalysis

Beatriz Mourino, Sauradeep Majumdar, Xin Jin, Fergus McIlwaine, Joren Van Herck, Andres Ortega-Guerrero, Susana Garcia and Berend Smit*

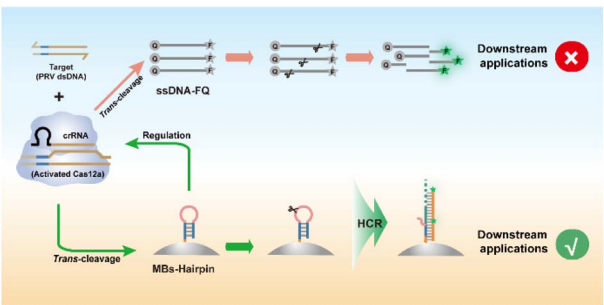
11447



Inter-cluster-linker-absence-enabled sub-Ångstrom pore modulation in a metal–organic framework for multi-scenario CO_2 capture

Jia-Wen Wang, Shu-Cong Fan, Wenyu Yuan, Ying Wang and Quan-Guo Zhai*

11456



Regulating CRISPR/Cas12a trans-cleavage on the hairpin DNA–MB nanointerface for enhanced multiplexed sensing application

Chenxi Zhao, Lijie Du, Dike Jiang, Jing Hu* and Xiandeng Hou*

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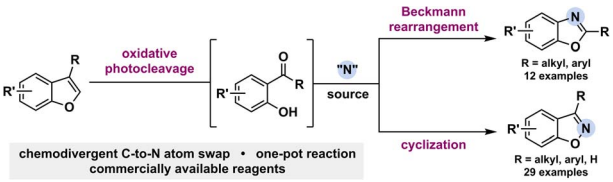
EDGE ARTICLES

11464

Chemodivergent C-to-N atom swap from benzofurans to benzisoxazoles and benzoxazoles

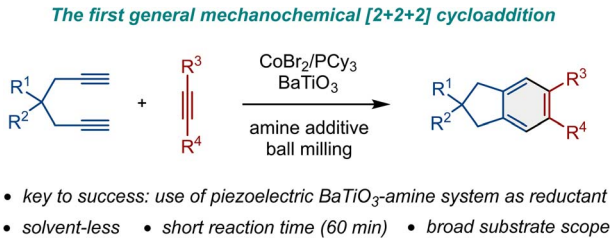
Ann-Sophie K. Paschke, Stefanie Schiele, Camille Pinard, Filippo Sandrini and Bill Morandi*



11468

A mechanochemical [2+2+2] cycloaddition facilitated by a cobalt(II) catalyst and piezoelectric materials

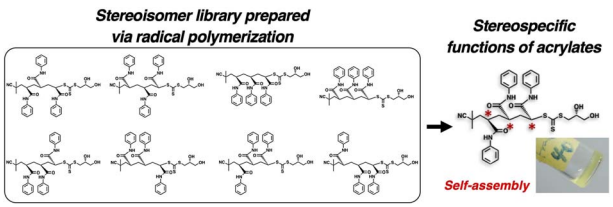
Kalipada Jana, Koji Kubota* and Hajime Ito*



11475

Stereoisomer library prepared *via* controlled radical polymerization: isolation, structural identification and discovery of stereospecific gelation behaviour of tri(N-phenyl acrylamide)

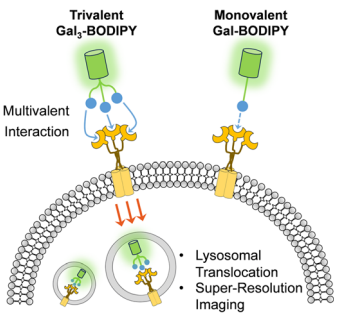
Yukiko Nagai, Hinako Iwamoto, Satoki Fukuda, Sotaro Akashi, Shota Iseri, Hayato Tada, Tomohiro Yamanaka, Konosuke Wada, Sotaro Tsuji, Toshikazu Ono, Yoshiko Miura, Tohru Taniguchi and Yu Hoshino*



11481

A BODIPY-tagged trivalent glycocluster for receptor-targeting fluorescence imaging of live cells

Chen Guo, Fang-Yu Si, Chen-Han Wang, Ning Wang, Xi-Le Hu, Tony D. James,* Jia Li,* Chengyun Wang* and Xiao-Peng He*



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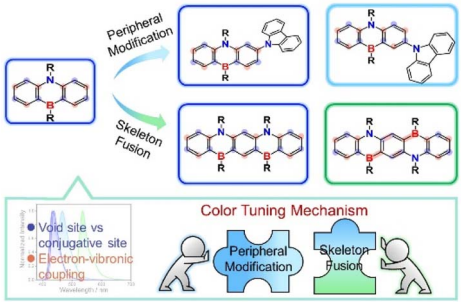
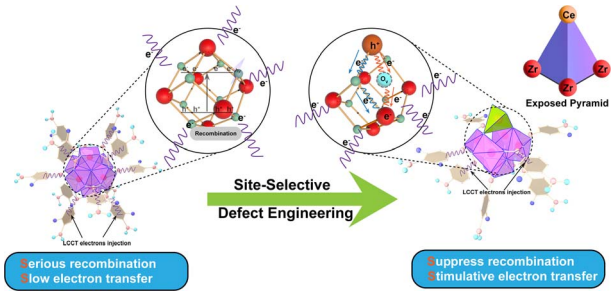


The color-tuning mechanism in multi-resonance thermally activated delayed fluorescence emitters: site effects in peripheral modification and skeleton fusion

Zicong Situ, Xingqing Li, Shengsheng Wei, Xiang Wang, Yang Li, Yan Wan, Lian Duan,* Andong Xia* and Zhuoran Kuang*

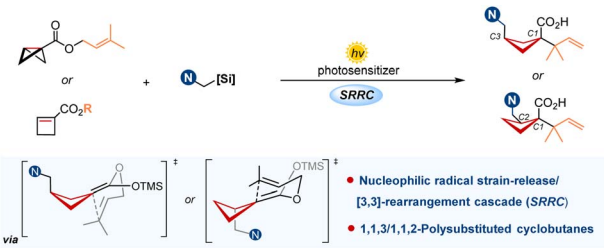
11498



Site-selective ligand defects open up a Zr-oxo cluster electron transfer pathway for CO_2 photoreduction

Yuhang Qi, Yiqiang He, Yuxin Liu, Zhe Zhang, Chunguang Li, Fanchao Meng, Shiyu Wang, Xiaobo Chen, Zhan Shi* and Shouhua Feng

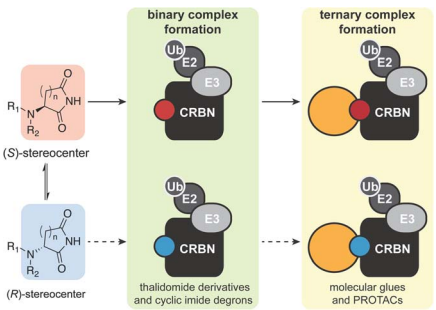
11508



Synthesis of polysubstituted cyclobutanes through a photoredox strain-release/[3,3]-rearrangement cascade

Fangqing Zhang, Chun Xu, Zichun Zhang, Zhuang Yang, Tao Peng, Wen Shao,* Xiaoming Feng* and Yangbin Liu*

11519



The contribution of cyclic imide stereoisomers on cereblon-dependent activity

Yuka Amako, Saki Ichikawa, Hannah C. Lloyd, N. Connor Payne, Zhi Lin, Andrew S. Boghossian, Matthew G. Rees, Melissa M. Ronan, Jennifer A. Roth, Qian Zhu, Bogdan Budnik, Ralph Mazitschek and Christina M. Woo*

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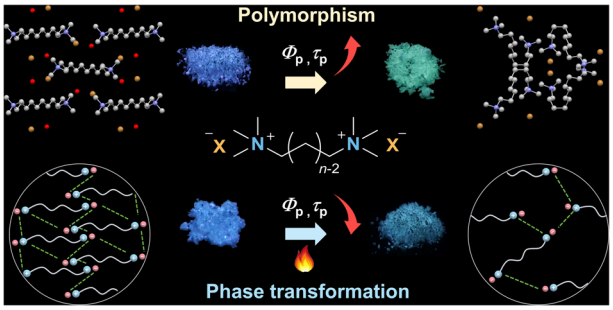
EDGE ARTICLES

11530

Polymorphism and phase transformation tuned luminescence and mechanistic insights in nonconventional luminophores

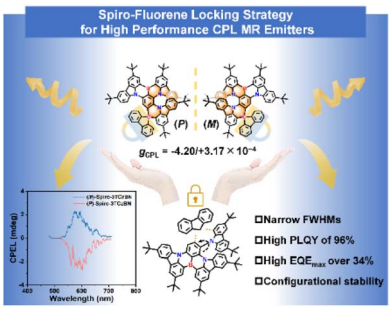
Anze Li, Zihao Zhao, Guangxin Yang, Qiang Zhang, Xiang Chen and Wang Zhang Yuan*



11539

Spiro-fluorene locked multi-resonance delayed fluorescence helical framework: efficient circularly polarized electroluminescent materials

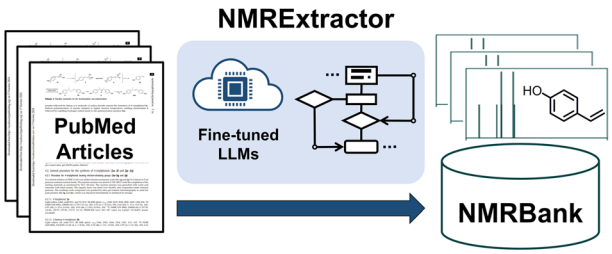
Xinliang Cai, Jinbei Wei,* Zhiqiang Li, Yexuan Pu, Youwei Wu and Yue Wang*



11548

NMRExtractor: leveraging large language models to construct an experimental NMR database from open-source scientific publications

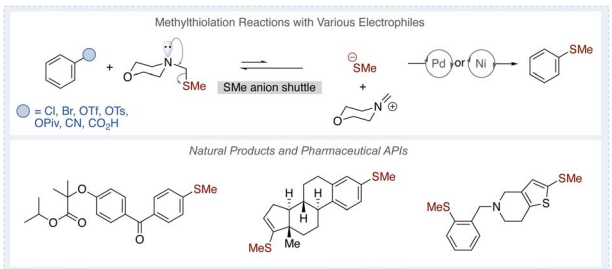
Qinggong Wang, Wei Zhang, Mingan Chen, Xutong Li, Zhaoping Xiong, Jiacheng Xiong,* Zunyun Fu* and Mingyue Zheng*



11559

Metal-catalyzed methylthiolation of chloroarenes and diverse aryl electrophiles

Sae Toyoda, Keiichiro Iizumi and Junichiro Yamaguchi*



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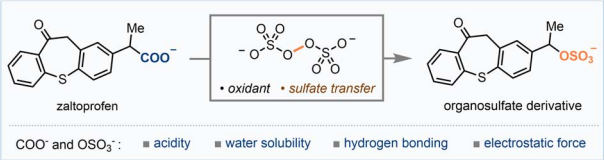
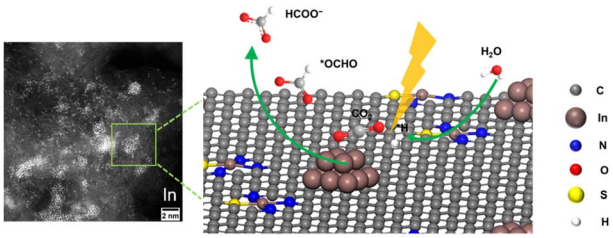
11568



Decarboxylative sulfation by persulfates

Zhen Xia, Ting Deng, Chunlan Song and Jiakun Li*

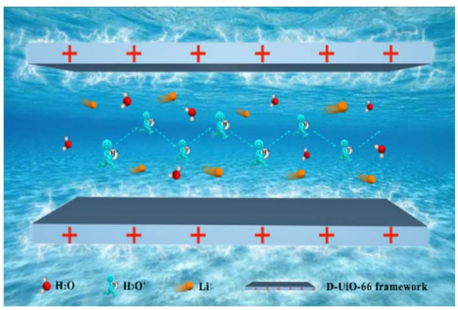
11574



Synergistic catalysis between In single atoms and In nanoparticles for highly selective electrocatalytic CO_2 reduction to formate with high current densities

Yuxin Chen, Junyoung Choi, Fangkui Liang, Xinyi Tan,* Yudi Chen, Jiahui Yang, Song Hong, Xin Zhang, Alex W. Robertson, Yousung Jung* and Zhenyu Sun*

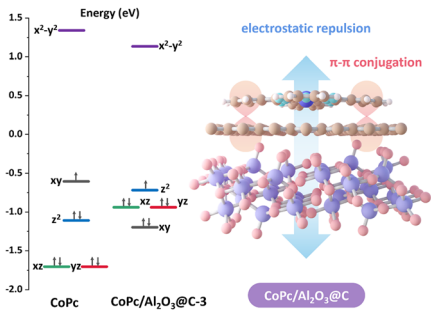
11581



Synergistic chaotropic effect and defect engineering promoting ultrahigh ionic conductivity in MOFs

Dongbo Liu, Xiao-Min Li,* Junchao Jia, Xingyu Long, Junpeng Yan, Mengyang Xiao, Aziz Bakhtiyarovich Ibragimov and Junkuo Gao*

11587



Engineering catalyst–support interactions in cobalt phthalocyanine for enhanced electrocatalytic CO_2 reduction: the role of graphene-skinned Al_2O_3

Qianqian Bai, Bingyun Ma, Le Wei, Mutian Ma, Zhangyi Zheng, Wei Hua, Zhenyang Jiao, Min Wang, Huihong Yuan, Zhihe Wei, Tao Cheng, Xiaoxing Ke, Jun Zhong, Fenglei Lyu,* Zhao Deng* and Yang Peng*

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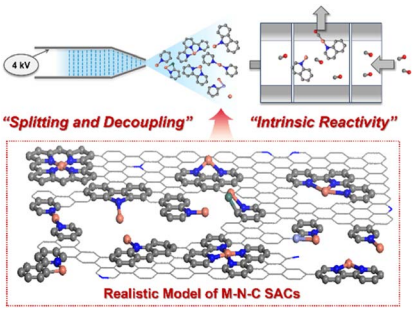
11598

Unraveling the local coordination effect of Cu–N–C single-atom catalysts towards CO adsorption *via* a gas-phase cluster model approach

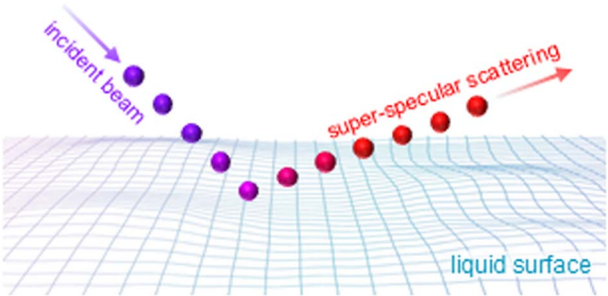
Qing Wang, Dingding Lv, Jian Zhou, Detong Kong, Shanshan Lin, Lili Zhang, Zhen-an Qiao, Yuxiao Ding* and Xiaoyan Sun*



11608

Molecular beam scattering of neon from flat jets of cold salty water

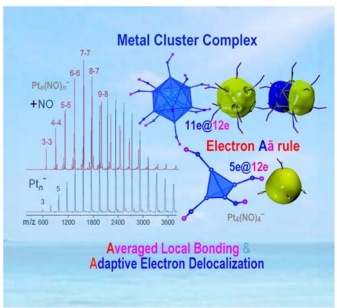
Walt Yang, Madison M. Foreman, Tiffany C. Ly, Kevin R. Wilson and Daniel M. Neumark*



11619

Privileged metal cluster complexes

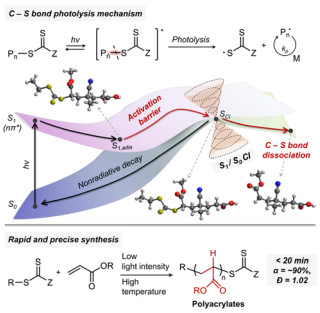
Shiquan Lin, Dan Li, Dandan Zhang, Lijun Geng, Yuhan Jia, Weizhe Wang, Longjiu Cheng,* Shiv N. Khanna and Zhixun Luo*



11626

Rapid and precise synthesis of acrylic polymers driven by visible light

Changhoon Yu, Jong-Kwon Ha, Mincheol Park, Jungwook Lee, Jinho Choi, Boyoung Y. Park, Cyrille Boyer,* Seung Kyu Min* and Min Sang Kwon*



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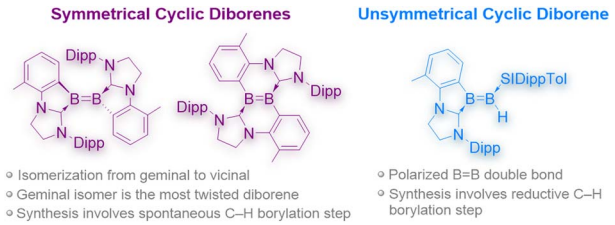
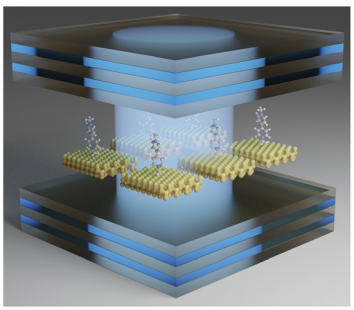
11637



Synthesis of symmetrical and unsymmetrical cyclic diborenes *via* NHC-directed C–H borylation

Cornelius Mihm, Sourav Kar, Andreas Sachs, Dario Duwe, Rian D. Dewhurst and Holger Braunschweig*

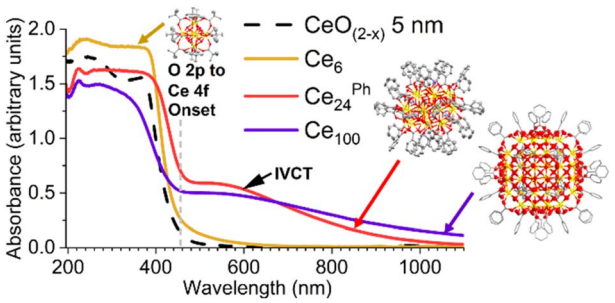
11644



Polariton mediated electron transfer under the collective molecule–cavity coupling regime

Eric R. Koessler,* Arkajit Mandal, Andrew J. Musser, Todd D. Krauss and Pengfei Huo*

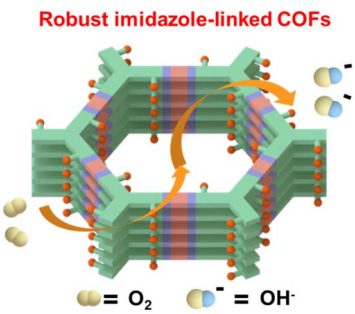
11659



Photoabsorption of 1–2 nm molecular Ce-oxo nanoclusters *versus* ceria: intervalence charge transfer but no size effects

Stephen E. Brown and Sebastian D. Pike*

11669



Amplification effect of side group regulation *via* imidazolate linkages of covalent organic frameworks for efficient oxygen reduction

Mengyuan Chen, Zhiqiang Zhu, Youxin Ji,* Xiangtao Kong, Diandian Han* and Lipeng Zhai*

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CORRECTIONS

11678

Correction: Hydroxy-directed iridium-catalyzed enantioselective formal β-C(sp^2)–H allylic alkylation of α,β-unsaturated carbonyls

Sankash Mitra, Rahul Sarkar, Aditya Chakrabarty and Santanu Mukherjee*

11679

Correction: Collective motions in the primary coordination sphere: a critical functional framework for catalytic activity of the oxygen-evolving complex of photosystem II

Hiroshi Isobe,* Takayoshi Suzuki, Michihiro Suga, Jian-Ren Shen and Kizashi Yamaguchi

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