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See Lauren Takahashi, Keisuke Takahashi *et al.*, pp. 15769–15780. Image reproduced by permission of Lauren Takahashi from *Chem. Sci.*, 2025, **16**, 15769.

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Mattia Silvi* and Claudia Bonfio*

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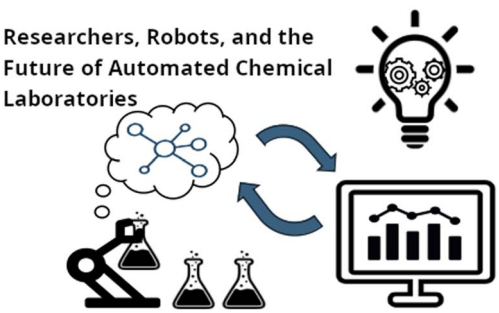
AI and automation: democratizing automation and the evolution towards true AI-autonomous robotics

Lauren Takahashi,* Mikael Kuwahara and Keisuke Takahashi*



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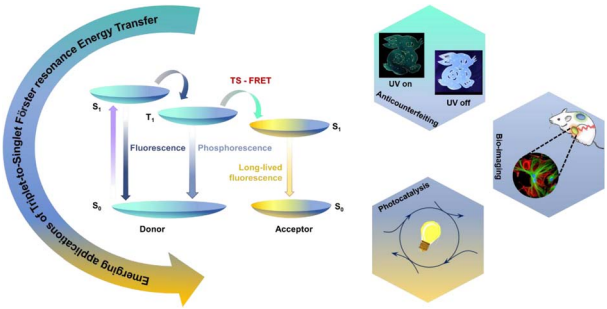
PERSPECTIVES

15781

Triplet-to-singlet FRET (TS-FRET) in pure organic phosphors: emerging applications and new opportunities

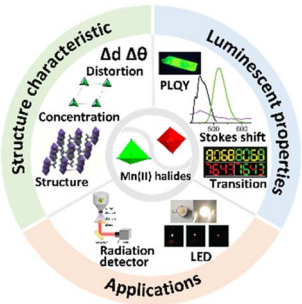
Sundaravalli Narayanan, Anju Ajayan Kongasseri and Subi J. George*



15796

Emission-tunable manganese(II) halides: structure–property relationships and functional applications

Chuying Wang, Yacong Li and Zhengtao Deng*

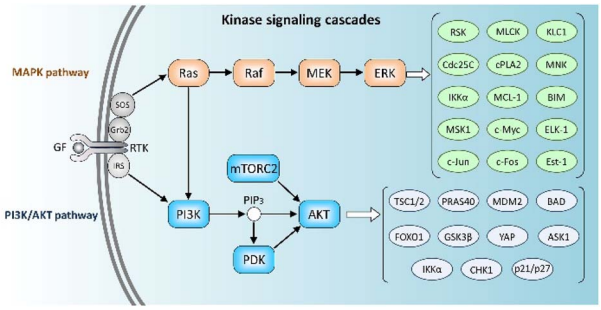


REVIEWS

15815

Kinase signaling cascades: an updated mechanistic landscape

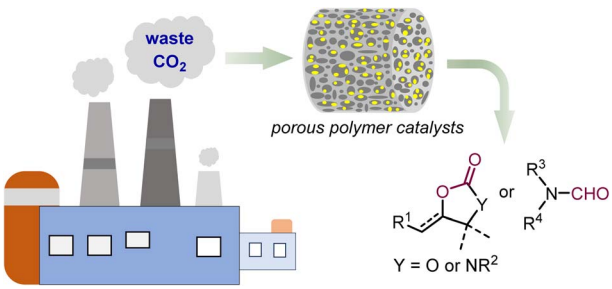
Ruth Nussinov,* Clil Regev and Hyunbum Jang



15836

Direct conversion of waste CO_2 over porous polymer catalysts

Jun-Song Jia, Ying Liang* and Ying-Ming Pan*



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REVIEWS

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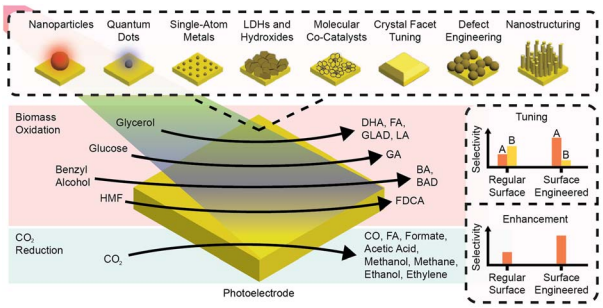

Surface engineering strategies for selectivity tuning and enhancement in photoelectrochemical biomass and CO_2 valorization

Yudhistira Tirtayasri Amrillah, Kaijian Zhu, Fani Rahayu Hidayah Rayanisaputri, Fita Widiyatun, Vivi Fauzia, Munawar Khalil, Fatwa F. Abdi* and Ferry Anggoro Ardy Nugroho*

EDGE ARTICLES

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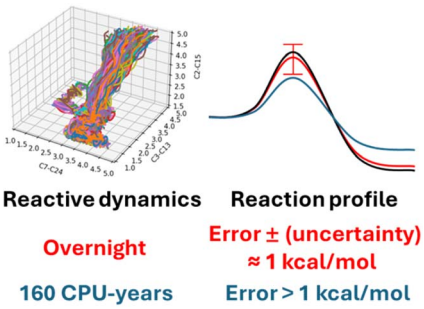
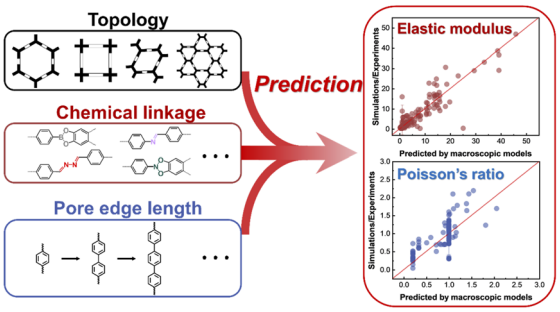


AIQM2: organic reaction simulations beyond DFT

Yuxinxin Chen and Pavlo O. Dral*

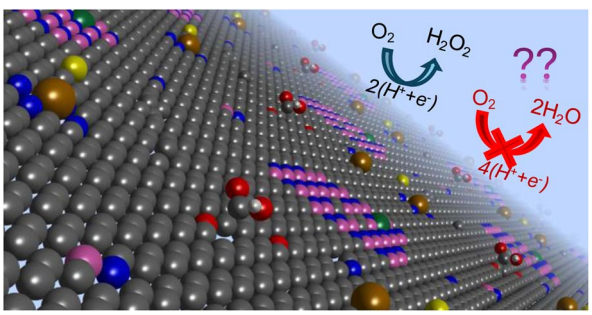
15913



Intrinsic mechanical properties of two-dimensional covalent organic frameworks

Liangtao Xiong, Chengbin Fu, Jiaxin Tian, Yubo Geng, Lixin Han, Han Zhang and Haoyuan Li*

15926



Selectivity trends in two-electron oxygen reduction: insights from two-dimensional materials

Samira Siahrostami*

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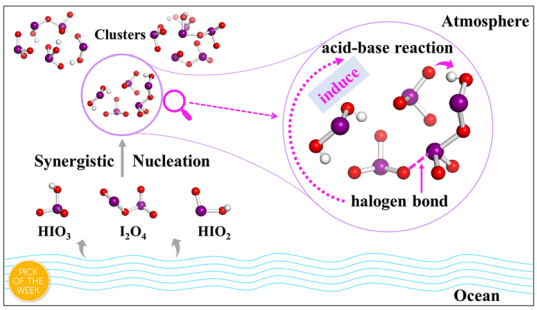
15935

Significance of halogen bonding in the synergistic nucleation of iodine oxoacids and iodine oxides

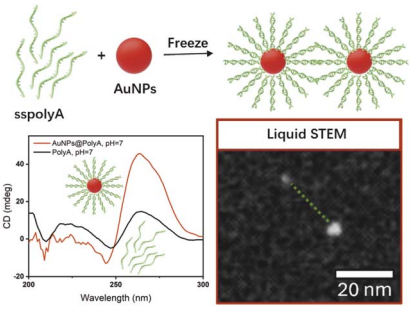
Rongjie Zhang, Yueyang Liu, Rujing Yin, Fangfang Ma, Deming Xia, Jingwen Chen, Hong-Bin Xie* and Joseph S. Francisco*



15947

Distinct structural interactions of polyadenine and polythymine on gold nanoparticles: from single strands to duplexes

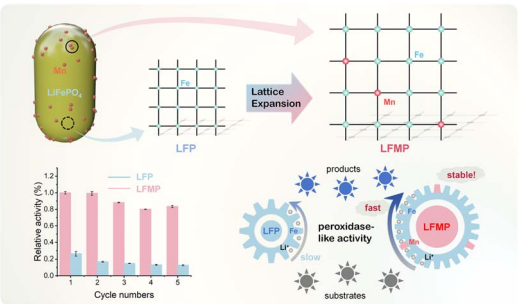
Manuel Núñez-Martínez,* Jinyi Dong, Isabel García,* Bjorn De Busschere, Nathalie Claes, Sara Bals* and Luis M. Liz-Marzán*



15955

Modulating ion migration realizes both enhanced and long-term-stable nanozyme activity for efficient microplastic degradation

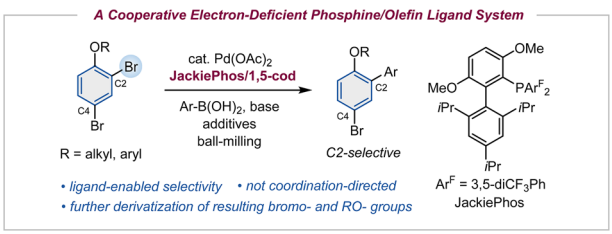
Pingping Wan, Guanghui Chen, Jinsong Fan, Wenlong Tan, Xu Li, Lang Chen and Kun Li*



15964

A cooperative electron-deficient phosphine/olefin ligand system for the site-selective mechanochemical Suzuki–Miyaura cross-coupling of 2,4-dibromoaryl ethers

Yunpeng Gao, Julong Jiang, Satoshi Maeda, Koji Kubota* and Hajime Ito*



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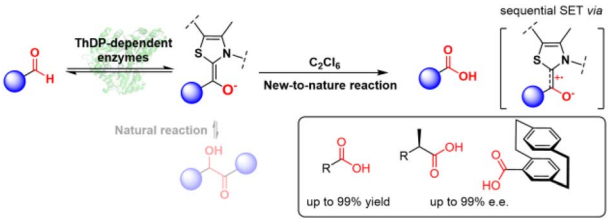
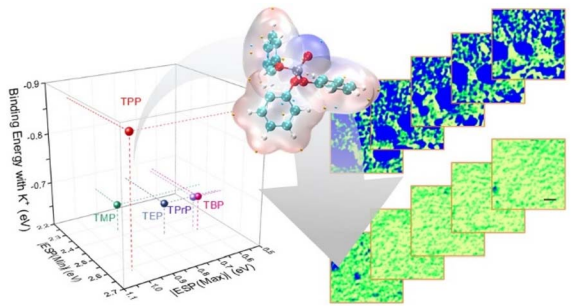


ThDP-dependent enzyme catalyzed oxidation of aldehydes

Xiaoyang Chen,* Meiting Zhou, Xinyu Duan, Yuting Zhang, Xiaohe Chu* and Jian Xu*

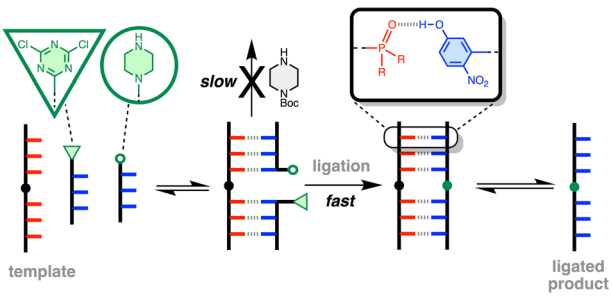
15982



Phosphorus-induced interfacial chemistry *via* electrolyte design for dense and highly stable potassium metal anodes

Junpeng Xie, Zhenjiang Yu, Jinliang Li, Qing Zhang, Wenjie Mai, Zhixin Tai,* Yajie Liu* and Zaiping Guo*

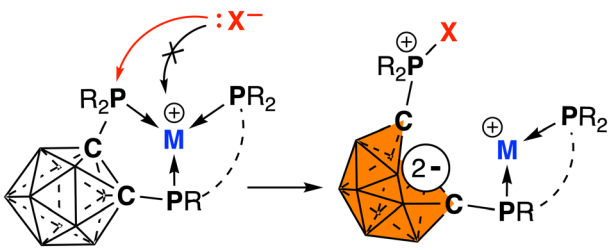
15991



Template-directed ligation of recognition-encoded melamine oligomers

Laura A. Beale, Joseph T. Smith, Cecilia J. Anderson, Oliver N. Evans and Christopher A. Hunter*

15997



Non-spectator behavior of a neutral phosphine ligand driven by a redox-active boron cluster

Jared R. Riffle, Cash L. Jowers, Sarah Luna, Mark D. Smith and Dmitry V. Peryshkov*

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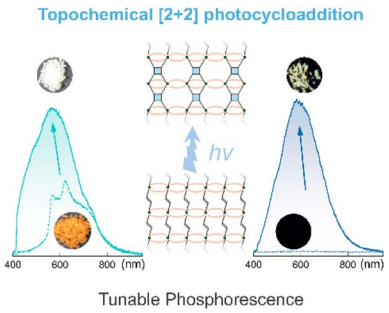
16004

Topochemical photocycloaddition in two-dimensional lead-halide coordination polymers with tunable phosphorescence

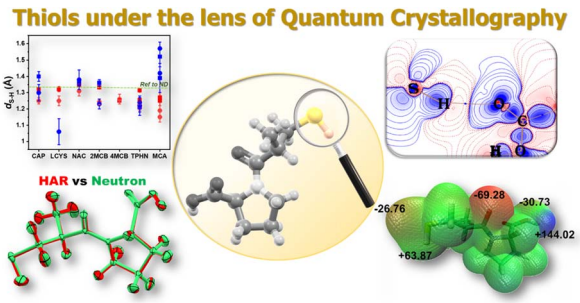
Zhongwei Chen, Jin Wu, Zeyu Deng,* Congcong Chen, Jianning Feng, Baixu Ma, Lizhi Tao, Lingling Mao and Haipeng Lu*



16016

Weak yet directional: supramolecular interactions of thiols unravelled by quantum crystallography

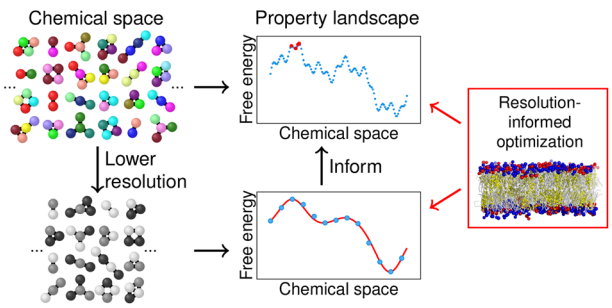
Ashi Singh, Kiran Avinash, Amit Kumar Pradhan, Aditya Kumar Prajapati, Alison J. Edwards and Sajesh P. Thomas*



16027

Navigating chemical space: multi-level Bayesian optimization with hierarchical coarse-graining

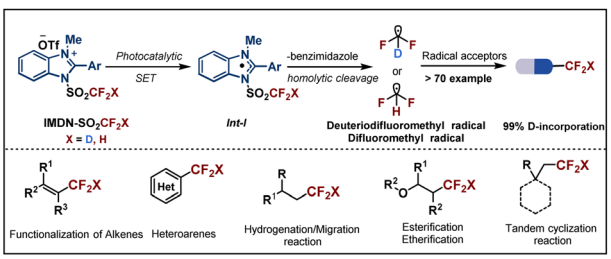
Luis J. Walter and Tristan Bereau*



16039

A practical photocatalytic strategy for radical (deuterio)difluoromethylation using imidazolium reagents

Chao Sun, Yinpu Shen, Heyin Li, Zhen Wang, Yifan Li, Mengjun Huang, Zhenlei Zou, Jing Liu, Ao Liu, Yi Pan, Weigang Zhang* and Yi Wang*



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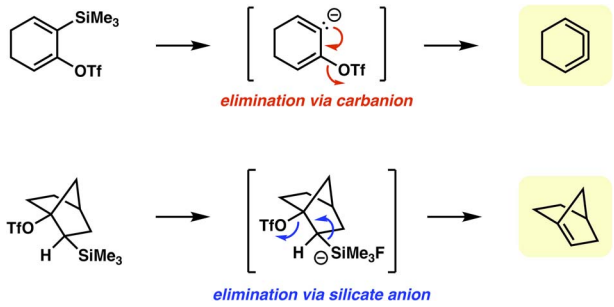
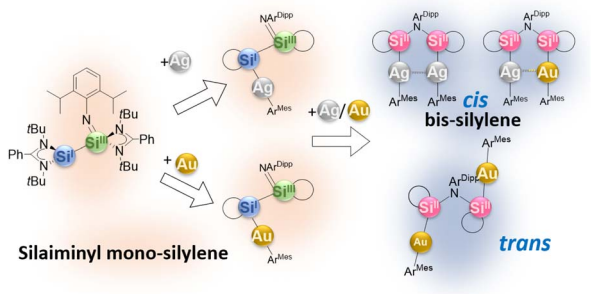


Mechanisms of Kobayashi eliminations for the generation of highly strained arynes, cyclic cumulenes, and anti-Bredt olefins

Zach G. Walters, Dominick C. Witkowski, K. N. Houk and Neil K. Garg*

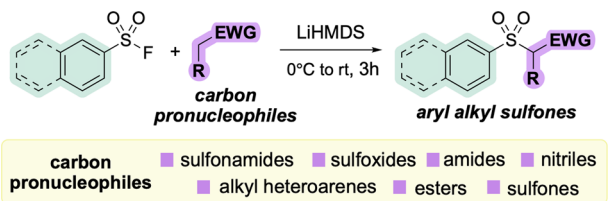
16057



On-demand switching from mono-silylene to bis-silylene to access mono-, di- and mixed coinage metal complexes

Xiaofei Sun,* Da Jin, Ravi Yadav, Frederic Kraetschmer, Ralf Köppe and Peter W. Roesky*

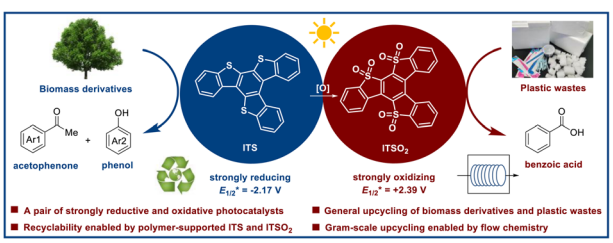
16063



Sulfur fluoride exchange with carbon pronucleophiles

Joseph R. Novicki,* Matthew D. Teeter, Neil J. Baldwin, Christopher W. am Ende, Thomas R. Puleo,* Alistair D. Richardson* and Nicholas D. Ball*

16070



A pair of strongly reductive and oxidative photocatalysts for the general upcycling of biomass derivatives and plastic wastes

Hao Cui, Xiang Chen, Xiong She, Wen-Xin Su, Shi-Chao Chen and Xiao Zhang*

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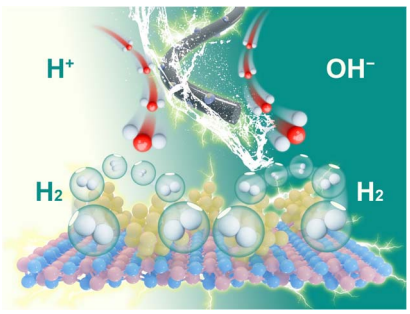
16081

Electronic metal–support interaction induces electron deficiency in iridium for promoted ampere-grade-current-density electrocatalytic hydrogen evolution

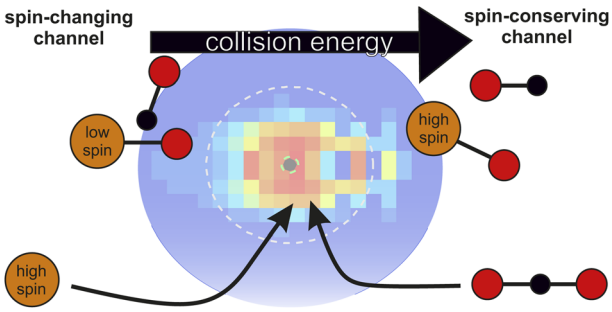
Linfeng Zhang, Weimo Li, Siyu Ren, Yue Zhang, Wei Song, Ce Wang and Xiaofeng Lu*



16090

CO_2 activation by gaseous zirconium cations: competition between spin-changing and spin-conserving pathways

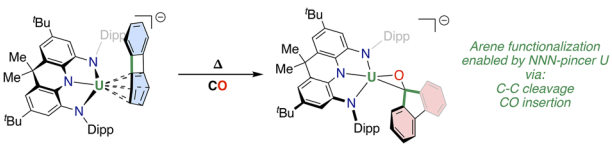
Marcel Meta, Yang Liu, Martin Wedele, Shaun G. Ard, Tucker W. R. Lewis, Milan Ončák, Nicholas S. Shuman, Albert A. Viggiano, Hua Guo* and Jennifer Meyer*



16101

C–C bond cleavage and carbonylation enabled by an NNN-pincer uranium scaffold *via* metal–arene interaction

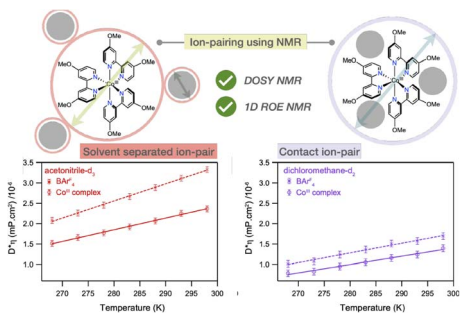
Yue Pang, Thayalan Rajeshkumar, Rosario Scopelliti, Laurent Maron* and Marinella Mazzanti*



16110

Probing the influence of ion-pairing on ligand-field excited-state dynamics

Atanu Ghosh, Daniel Holmes and James K. McCusker*



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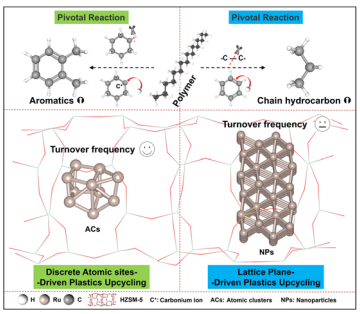
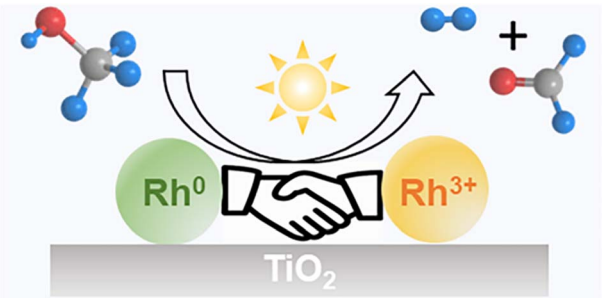
16121



Hydrogen/solvent-free plastic valorization *via* loosely coordinated ruthenium sites steering selective aromatization

Fan Mo, Qixing Zhou,* Pengfei Wang, Weitao Liu, Chuan Yin, Zelin Hou, Wendan Xue, Qi Wang, Jianling Wang, Tong Zheng, Zongxin Tao and Xiang Li

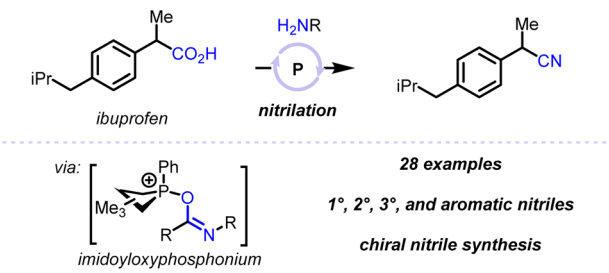
16137



Unlocking synergy between multi-valence rhodium species for promoted methanol photoreforming

Mu Xiao, Weizhen Meng, Yalong Jiao, Haijiao Lu, Zhiliang Wang, Guangyu Zhao, Zitong Wang, Yonggang Jin and Lianzhou Wang*

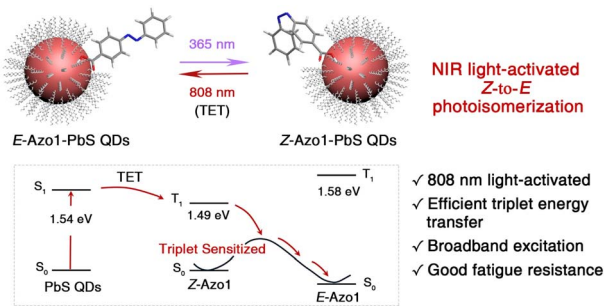
16145



Nitrilation of carboxylic acids by P^{III}/P^{V}-catalysis

Siraj Z. Ali, Nicolás A. Manno, Jeff Shen, Alessia Schenker, Jeffrey M. Lipshultz, Nicholas A. White* and Alexander T. Radosevich*

16151



Near-infrared light-activated *Z*-to-*E* isomerization of azobenzene *via* triplet sensitization from PbS quantum dots

Yanan Feng, Qingxin Luan, Shuai Zhang, Lin Xi, Shijie Zhang, Kezhou Chen, Tiegen Liu and Lili Hou*

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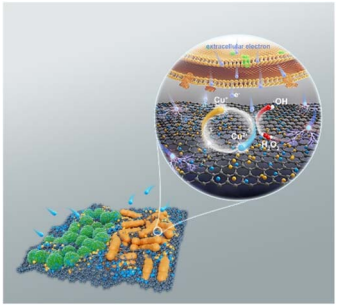
16158

Bacteria-driven bio-electroactive sterilization

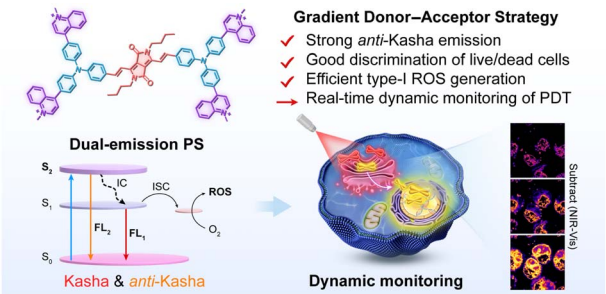
Mingming Qin, Qiuping Qian,* Xiaoqing Gao, Tianxi Shen, Feng Jia, Min Wu, Kelong Fan and Yunlong Zhou*



16168

Dual-emissive self-reporting photosensitizers characterized by Kasha/*anti*-Kasha behaviors engineered *via* a gradient donor–acceptor strategy

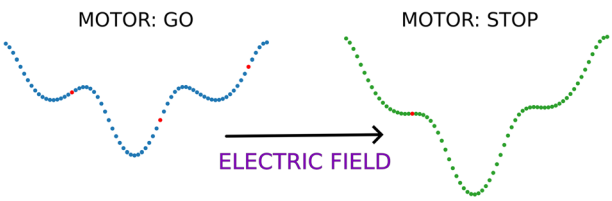
Xixin Gu, Xinyi Zhang, Yujie Han, Ju Mei,* Qi-Wei Zhang* and Jianli Hua*



16180

Controlling molecular machines *via* optimally oriented external electric fields

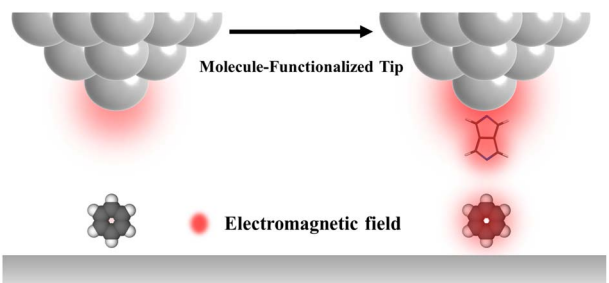
Marco Severi,* Ibério de P. R. Moreira, Jordi Ribas-Ariño, Wolfgang Quapp and Josep Maria Bofill



16187

Design of functionalized tips driven by m olecule–plasmon coupling

Huijie He, Xueyang Zhen, Shuang Li, Sibing Chen and Xing Chen*



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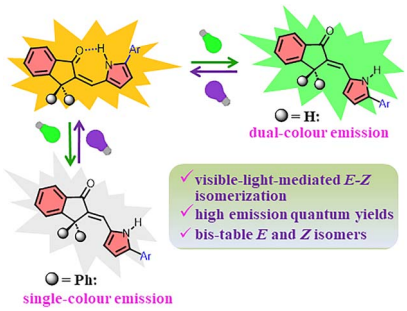
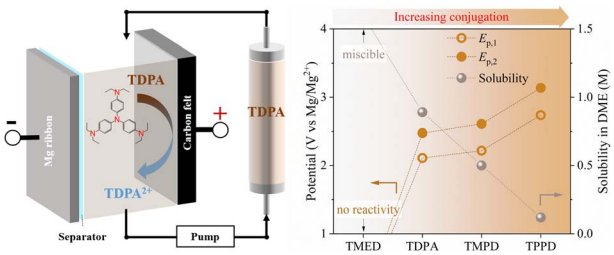
16196



Arylpyrrolylidene-indanones as readily synthesised photoswitches offering dual- and single-colour fluorescence toggling with nearly quantitative *E*/*Z* isomerisation under visible light

Satyajit Bera, Supriya Bhunia, Anirban Dolai, Sk Majid Box, Arpan Das and Subhas Samanta*

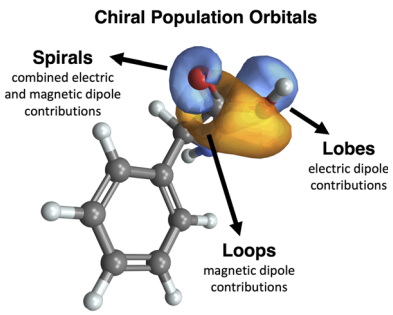
16205



Conjugation effect of amine molecules in non-aqueous Mg redox flow batteries

Yunan Qin, Vaidyanathan Sethuraman, Seong-Gyu Choi, Richard Gonzalez, Chengxiang Chen, Lei Cheng, Chao Luo* and Tao Gao*

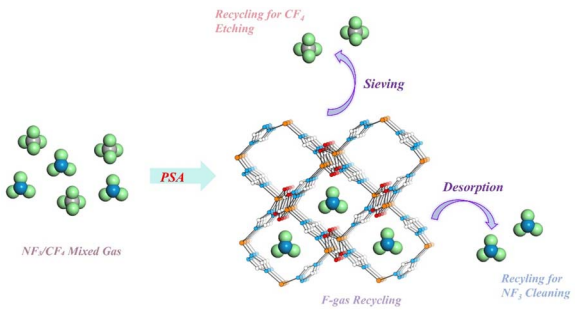
16218



Chiral population analysis: a real space visualization of X-ray circular dichroism

Victor M. Freixas,* Jérémy R. Rouxel, Sergei Tretiak, Niranjan Govind and Shaul Mukamel

16225



A scalable zinc-based coordination network for energy-efficient NF_3/CF_4 separation with unprecedented selectivity

Yi-Tao Li, Weilin Li, Li-Ping Zhang, Na Geng, Li Xu, Shao-Min Wang, Tingyu Zhu, Qingqing Guan,* Yangyang Guo,* Xingxing Li* and Qing-Yuan Yang*

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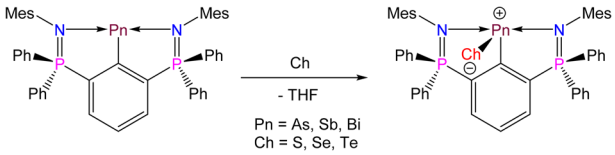
16232

Nature of the heavy formal double bonds As═Ch, Sb═Ch and Bi═Ch (Ch = S, Se, Te) in NCN-pincer supported arsinidene, stibinidene and bismuthinidene chalcogenides

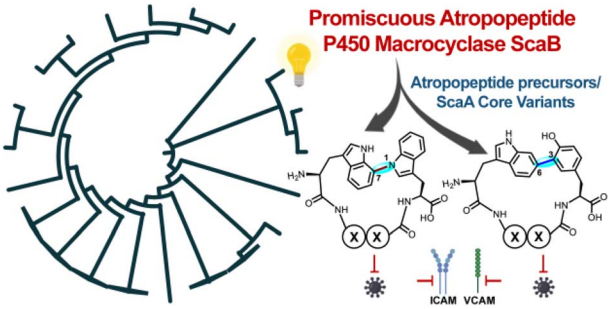
Fabio Meyer, Arina Siumbeli, Libor Dostál,* Emanuel Hupf* and Jens Beckmann*



16240

Phylogeny-guided discovery of a promiscuous P450 macrocyclase for the production of diverse atropopeptides

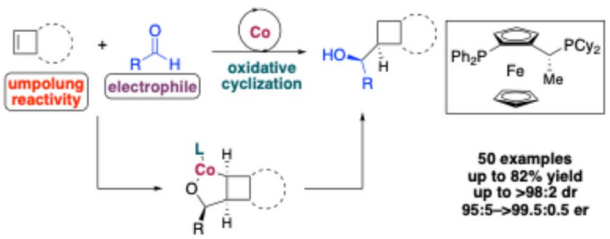
Bin Tan, Peter Breunig, Lamia Arbib, Yuya Kakumu, Friederike Biermann, Kornelia Hardes, Jasmin Hefendehl and Eric J. N. Helfrich*



16250

Cobalt-catalyzed diastereo- and enantioselective reductive coupling of cyclobutenes and aldehydes through umpolung reactivity

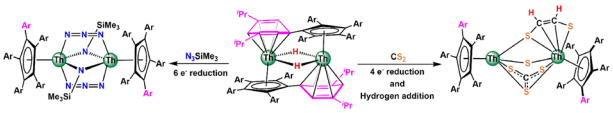
Chuiyi Lin, Jiwu Zhang, Zhihan Zhang,* Qinglei Chong* and Fanke Meng*



16259

Multi-electron redox reactivity of a thorium(II) hydride synthon

Xianghui Shi, Guorui Qin, Peng Deng, Iker Del Rosal, Laurent Maron* and Jianhua Cheng*



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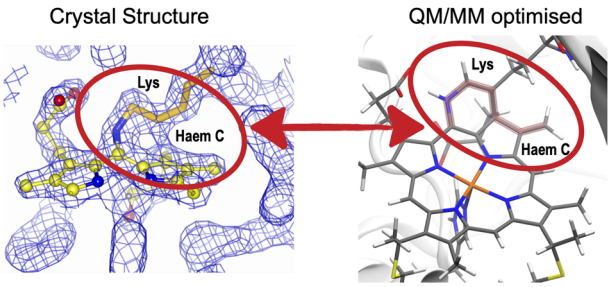
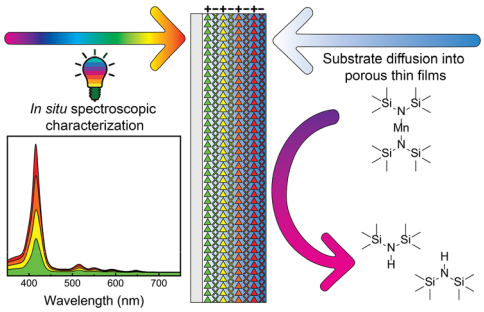
16266



Double crossed? Structural and computational studies of an unusually crosslinked haem in *Methylococcus capsulatus* cytochrome P460

Hans E. Pfalzgraf, Aditya G. Rao, Kakali Sen, Hannah R. Adams, Marcus Edwards, You Lu, Chin Yong, Sofia Jaho, Takehiko Tosha, Hiroshi Sugimoto, Sam Horrell, James Beilsten-Edmands, Robin L. Owen, Colin R. Andrew, Jonathan A. R. Worrall, Ivo Tews, Adrian J. Mulholland,* Michael A. Hough* and Thomas W. Keal*

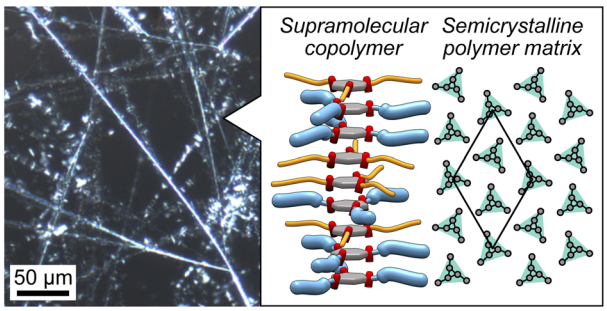
16284



***In situ* characterization of post-synthetic metalation in porous salt thin films**

Joe D. Simmons, Subham Sarkar, Andrew A. Ezazi, Aishanee Sur, Ethan T. Iverson, Merissa N. Morey, Austin D. Chivington, Sarah G. Fisher, Jaime C. Grunlan, David C. Powers* and Eric D. Bloch*

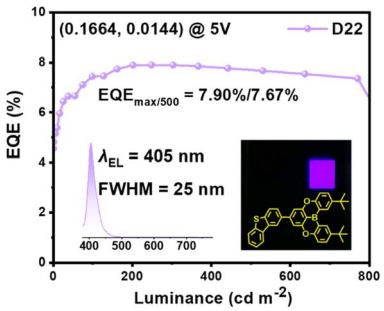
16293



Biasing the polymorphism of a semicrystalline covalent polymer by exploiting the microstructure of supramolecular copolymers

Alexi Riba-Bremerch, Arnaud Y.-G. Delplanque, Clément Guibert and Nathan J. Van Zee*

16304



Achieving high efficiency ultrapure violet OLEDs with a CIE$_y$ coordinate of below 0.015 through precise manipulation of peripheral heavy atom sulfur

Rui Chen, Shengyu Li, Hao Huang, Xingwen Tong, Yuchao Liu, Zhongjie Ren, Shian Ying,* Liqun Liu* and Shouke Yan*

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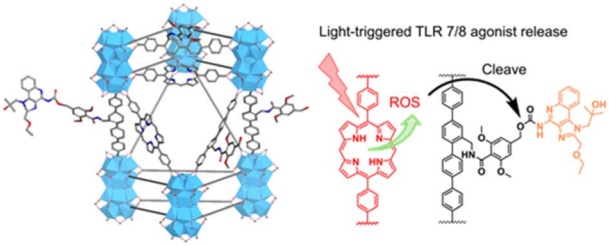
16314

Light-triggered toll-like receptor activation in a nanoscale metal–organic framework for synergistic PDT and cancer immunotherapy

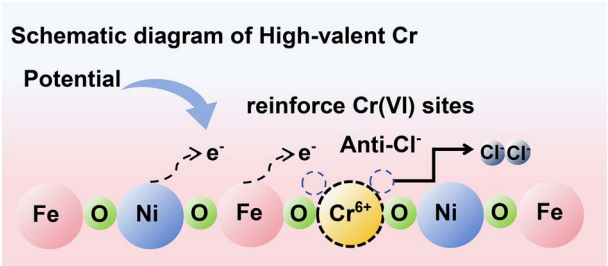
Yibin Mao, Langston Tillman, Xiaomin Jiang, Wangqing Bian, Chaoyu Wang, Tobias Fromme, Ralph R. Weichselbaum and Wenbin Lin*



16321

Stabilizing NiFe active sites using a high-valent Lewis acid for selective seawater oxidation

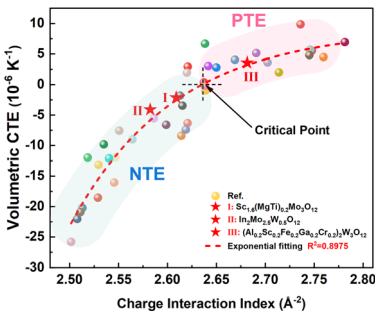
Chenxi Liu, Zefeng Teng, Xu Liu, Rui Zhang, Jingqi Chi,* Jiawei Zhu, Junfeng Qin,* Xiaobin Liu, Zexing Wu and Lei Wang*



16331

Predicting thermal expansion in framework compounds using a charge interaction index

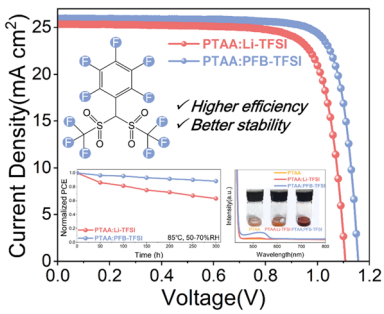
Xin Chen, Qilong Gao,* Kaiyue Zhao, Yongqiang Qiao, Andrea Sanson, Qiang Sun, Juan Guo, Shogo Kawaguchi, Erjun Liang and Jun Chen



16339

A non-ionic fluorinated p-dopant enables the construction of efficient and stable perovskite solar cells

Zhongquan Wan,* Wang Yu, Jinyu Yang, Yunpeng Zhang, Yuanxi Wang, Runmin Wei, Muhammad Azam, Junsheng Luo* and Chunyang Jia*



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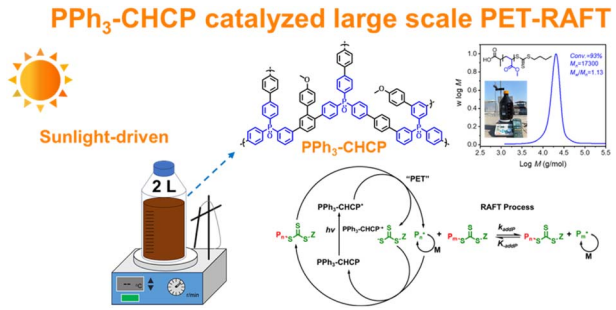
16347



Sunlight-driven photoinduced electron/energy transfer-reversible addition-fragmentation chain transfer polymerization at a large scale

Zi-Hui Fan, Wei-Wei Fang, Yi-Xing Liu, Zheng-Hao Xiao, Jian-Kun Yu, Xu-Yi He, Xian-Zhen Wang, Xue-Ning Tang, Lei Xia,* Long-Xiang Tang* and Tao He*

CORRECTION

16355

Correction: Unveiling the role of cobalt in the product regulation for CO_2 hydrogenation to light olefins over alumina-supported Co–Fe catalysts

Zhihao Liu, Wenlong Song, Peipei Zhang, Jiaming Liang,* Chengwei Wang, Chufeng Liu, Hanyao Song, Baojian Chen, Kangzhou Wang,* Guangbo Liu, Xiaoyu Guo, Yingluo He, Xinhua Gao, Jianli Zhang, Guohui Yang and Noritatsu Tsubaki*

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