

IN THIS ISSUE

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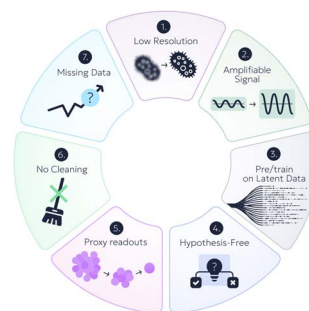
Inside cover
See Montree Sawangphruk et al., pp. 8453–8471. Image reproduced by permission of Montree Sawangphruk from *Chem. Sci.*, 2026, 17, 8453.

PERSPECTIVE

8327

Black-box data: a new paradigm for biomedicine in the AI era

Luca Naef* and Michael Bronstein*

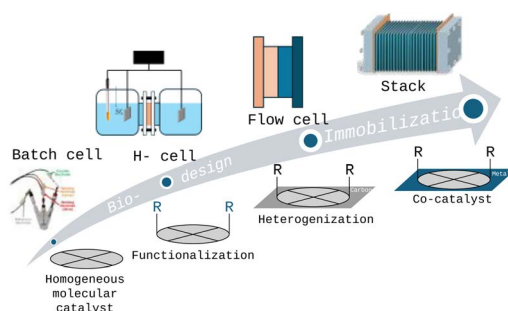


REVIEWS

8345

Molecular engineering of metalloporphyrins and phthalocyanines for homogeneous and heterogeneous CO₂ electroreduction

Aakash Santra, Arnab Ghatak, Zhiyuan Chen, Jing Shen, Joost Helsen, Yuvraj Birdja, Ally Aukauloo* and Chanjuan Zhang*



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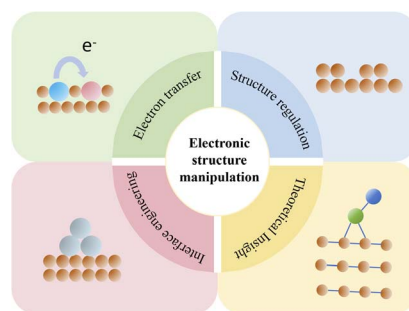
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REVIEWS

8372

Electronic structure manipulation in electrocatalysis: mechanisms and design principles

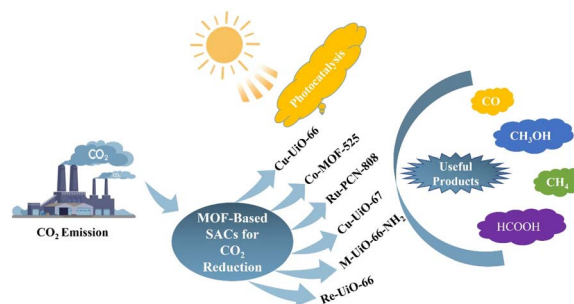
Hangkai Shi, Yuanduo Li, Shuyi Pang, Aixin Ma, Jianping Lai* and Lei Wang*



8396

Recent advances in MOF-based single-atom photocatalysts for CO₂ to solar fuel conversion under sunlight irradiation

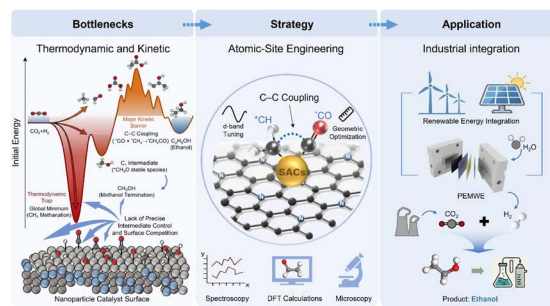
Adnan Majeed, Minh-Khoa Duong, Van-Duc Nguyen and Trong-On Do*



8432

Atomic-level engineering of single-atom catalysts for selective C–C coupling in CO₂ hydrogenation to ethanol

Wenyu Zheng, Yiming Liu, Xiaohai Zhang, Shengjie Bai,* Aobing Li, Kelun Jiang, Feng Wang, Ya Liu,* Yubin Chen and Shaohua Shen

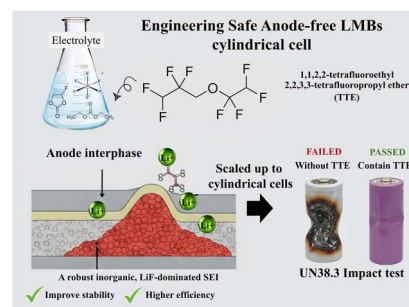


EDGE ARTICLES

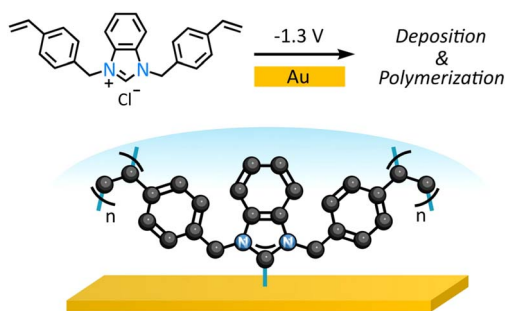
8453

Solvation-driven interphase engineering and mechanical failure pathways in large-scale anode-free lithium metal batteries

Nattanon Joraleechanchai, Nuttida Matkhaw, Thitiphum Sangsanit, Worapol Tejangkura and Montree Sawangphruk*



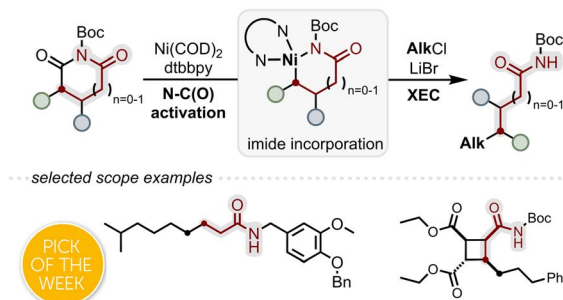
8472



Combined electrodeposition and electropolymerization method to produce surface-bound polystyrenyl NHC thin films

Jessica L. Bosso, Justin T. Lomax, Garima Garg, Wai-Tung Shiu, Jordan N. Bentley, Matthew J. Turnbull, Monika R. Snowden, James J. Noël,^{*} Cathleen M. Crudden,^{*} Joe B. Gilroy^{*} and Paul J. Ragogna^{*}

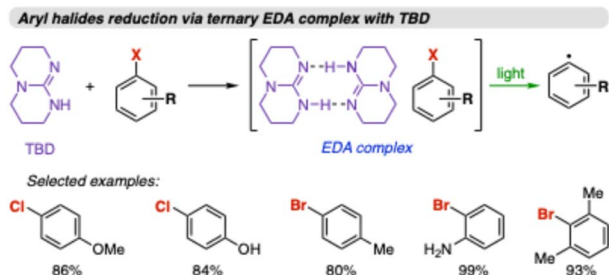
8479



Ring-opening decarbonylative C(sp³)-C(sp³) cross-electrophile coupling of cyclic imides with unactivated alkyl chlorides

Niklas J. Lentelink, Peter M. F. Pânzar, Nathalie A. V. Rowlinson and Bill Morandi^{*}

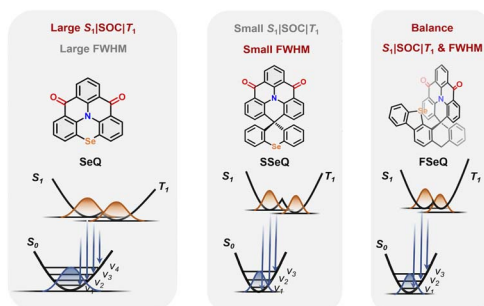
8486



Photochemical reduction of aryl chlorides, bromides, and iodides via ternary EDA complexes with guanidine bases

Robert J. Hannan, Alexandria M. Vondran, Sunghwan Cho, Kerry M. Hanson, Claire Tonnelé, David Casanova, Christopher J. Bardeen and Ana Bahamonde^{*}

8493



Theoretical insights into site-specific heavy-atom effects on MR-TADF emitters: modulation of spin-orbit coupling and color purity

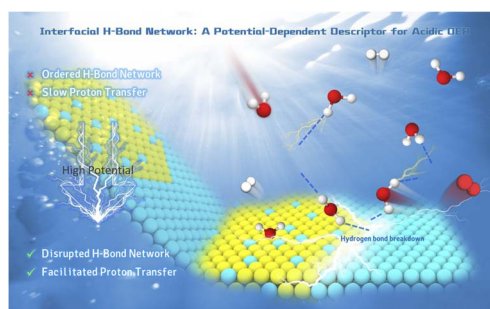
Shi-Jie Ge, Jian-Rong Wu and Zuo-Quan Jiang^{*}



8504

Engineering the interfacial water microenvironment to accelerate proton transfer for acidic oxygen evolution at high-potential

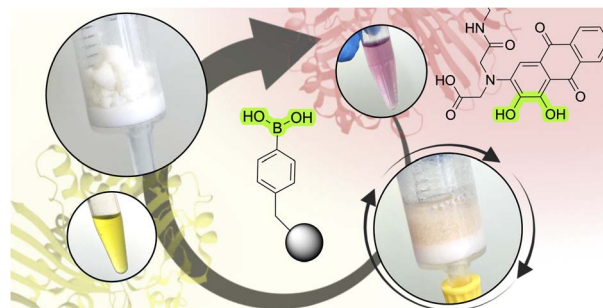
Xiaolong Liang, Ke Xu, Hengkun Yu, Xu Ge, Zhiwen Liu, Xueliang Mu, Shaokai Zhang, Jake M. Yang and Jinxuan Liu*



8513

Going full circle: dynamic covalent enzyme immobilisation via visually trackable boronate esters

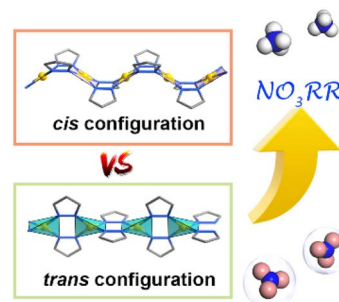
Glenn Bojanov, Juliette Swit and Francesca Paradisi*



8521

Polymorphism-driven coordination geometry engineering for boosting nitrate electroreduction in Cu-pyrazolate chains

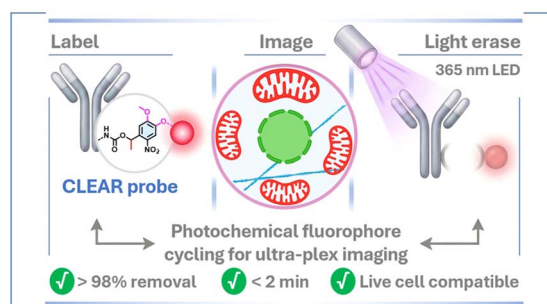
Zhanning Liu,* Shanna An, Qingzhong Xue* and Jian Tian*



8528

Optically switchable CLEAR probes enable rapid, biocompatible and high-efficiency fluorophore exchange for ultra-plex, high-resolution immunofluorescence imaging

Simanta Kalita, Pratibha Kumari, Arka Som, Srishti Mandal, Resmi V. Nair, Saswata Bandyopadhyay, Sushma Rao, Sudha Kumari and Sarit S. Agasti*



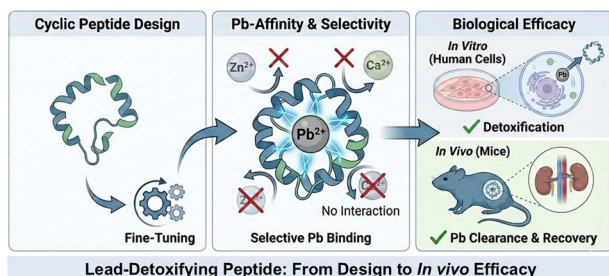
8542



Simulating enzyme catalysis with electrostatically embedded machine learning potentials

Valentin Gradisteanu, Elliot W. Chan, Lester Hedges, Meritxell Malagarriga, Rolf David, Miguel de la Puente, Damien Laage, Iñaki Tuñón, Marc W. van der Kamp* and Kirill Zinovjev*

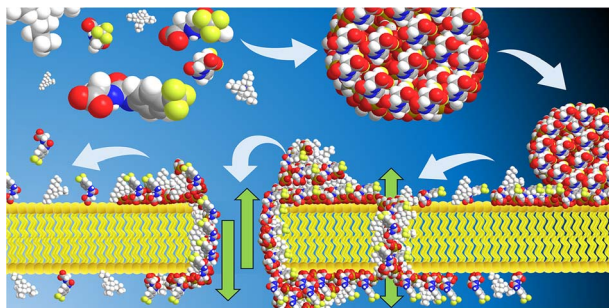
8557



Single stereocenter inversion of a cyclic tetrapeptide enables the detoxification of lead-exposed mice

Tagwa A. Mohammed, Luca Sauser, Erica Pedron, Yaël A. Hodel, Tadeáš Kalvoda, Francesco Prisco, Lubomír Rulišek, Jason P. Holland* and Michal S. Shoshan*

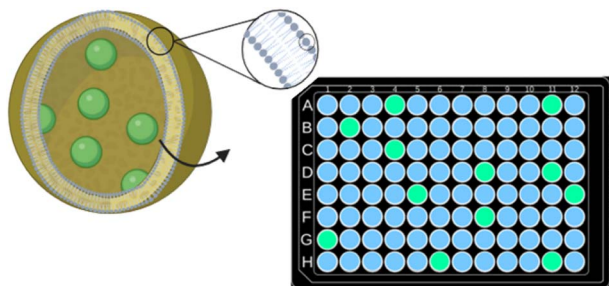
8567



Amino acid appended supramolecular self-associating amphiphiles demonstrate dual activity against both MRSA and ovarian cancer

Precious I. A. Popoola, Thomas L. Allam, Rebecca J. Lilley, Chandni Manwani, Olivia B. Keers, Junyang Tan, Kylie Yang, Yifan Long, Ewan R. Clark, Lisa J. White, Kira L. F. Hilton, Jennifer Rankin, Jennifer Baker, Charlotte Bennett, Hollie B. Wilson, Evelyn R. Morton, Alvaro Keskküla, Bethany Martin, Christopher O'Connor, J. Mark Sutton, Charlotte K. Hind,* Michelle D. Garrett,* Cally J. E. Haynes* and Jennifer R. Hiscock*

8580



An increased throughput workflow to identify ion transport and membrane lysis agents for antimicrobial discovery

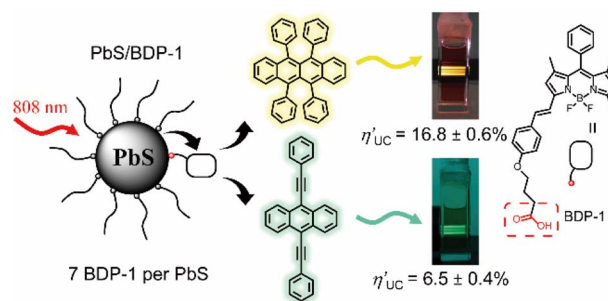
Kylie Yang, Caleb Marsh, Lisa J. White, Fergus W. Molyneux, Thomas L. Allam, Precious I. A. Popoola, Olivia B. Keers, Matthew Rice, Kira L. F. Hilton, Hiral A. Kotak, J. Mark Sutton, Jose L. Ortega-Roldan, Charlotte K. Hind,* Jennifer R. Hiscock* and Cally J. E. Haynes*



8595

Efficient near-infrared-excitable quantum dot-based triplet–triplet annihilation upconversion with a record anti-Stokes shift *via* low coverage of mono-styryl-BODIPY ligands

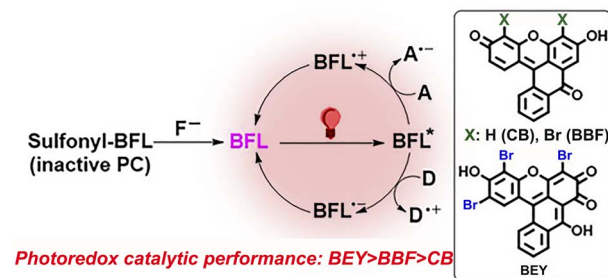
Ran Li, Lin-Han Jiang, Lin Xi, Ming-Yu Zhang, Hong-Juan Feng, Dong-Xue Guo, Lili Hou, Ling Huang* and Dai-Wen Pang*



8604

Red-light photoredox catalysis with bridged fluorescein derivatives: mechanistic insights and application to fluoride-responsive photopolymerization

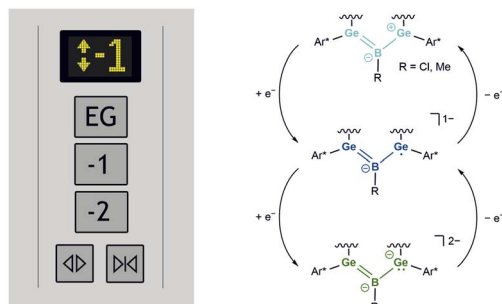
Dokyeong Lee, Hoyun Kim, Byunghyuck Jung, Sung Ho Yang, Hong-In Lee* and Jungkyu K. Lee*



8622

Three reversibly interconvertible redox states of boradigermaallyl: syntheses of radical allyl anion and allyl dianion

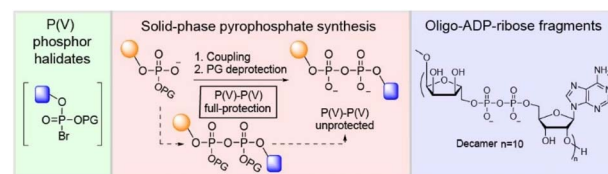
Stefan F. Mieke, Klaus Eichele, Hartmut Schubert, Holger F. Bettinger, Christian P. Sindlinger* and Lars Wesemann*



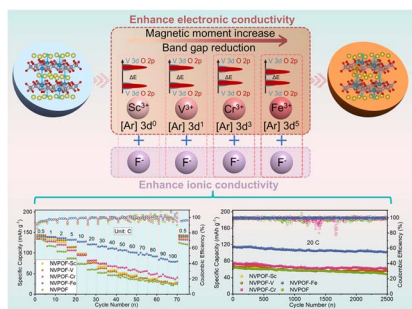
8630

Fully protected pyrophosphates *via* phosphorobromidates for the synthesis of biopolymers

Sven Wijngaarden, Femke L. A. M. van der Heijden, Koen J. Rijpkema, Bob van Puffelen, Nico J. Meeuwenoord, Danicia Ramcharan, Gijsbert A. van der Marel, Jeroen D. C. Codée, Herman S. Overkleeft and Dmitri V. Filippov*



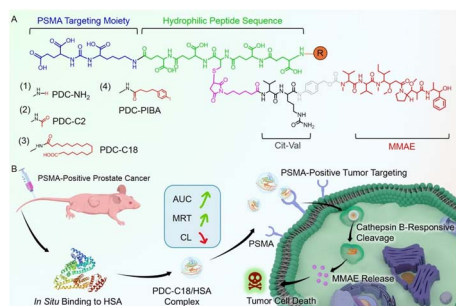
8638



Spin-regulated d–p hybridization enables high energy density and wide temperature operation of $\text{Na}_3\text{V}_2(\text{PO}_4)_2\text{F}$ -type cathodes for sodium-ion batteries

Qiang Fu, Qin He, Fangxiang Song, Xianquan Ao,*
Hanxiao Liu, Yang Cao, Rong Li,* Keliang Wang, Jing Li,
Cuiqin Li and Yao Xiao*

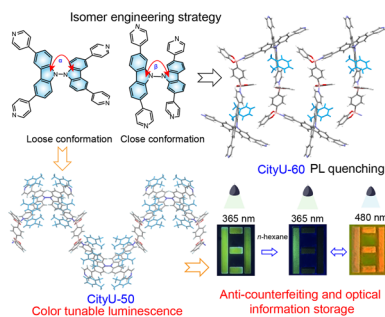
8651



Stearic acid-modified PSMA-targeting peptide–drug conjugate for long-acting prostate cancer therapy

Ziwen Qiu, Xiaorui Zheng, Shoumei Pan, Yingtao Zhong,
Xiayun Chen, Xuejun Wen, Xin Chen,* Shiyong Li,*
Hong Cheng* and Xiaoyuan Chen*

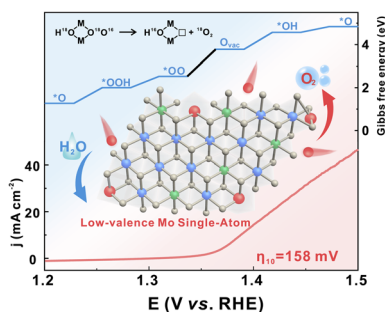
8662



Realizing luminescent single crystals of covalent organic polymers with color-tunable emission through isomer engineering

Yanyan Qin, Pengfei She,* Xiaoda Wang, Jianjun Wu,
Mingbing Lian, Feiyang Li, Shujuan Liu, Qianfeng Gu,
Yun Ma,* Qiang Zhao* and Qichun Zhang*

8670



Low-valent Mo single atoms stabilized by electronegative oxygen coordination enable efficient water oxidation

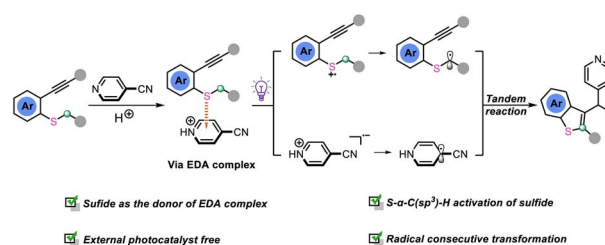
Yang Yang,* Ji-Kai Li, Qian-Nan Yang, Yi-Bin Yang,*
Jian-Hua Meng, Lin Zhang, Ying-Dan Wu, Ke-Xiang Wang,
Huan Chen, Zhi-Yuan Jiang, Rui Chao, Wei-Tao Wang,
Xiao Ma* and Zhao-Tie Liu*



8683

Photoinduced intramolecular S- α -C(sp³)-H functionalization enabled by an electron donor-acceptor complex-Mediated radical relay

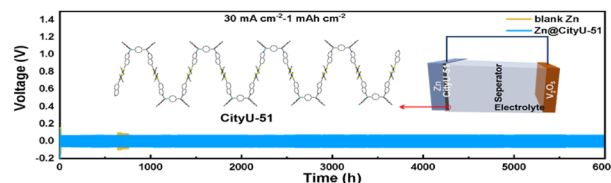
Tiantian Xu, Ran Hong, Tong Lu, Denghua Zhu, Jiong Yu, Min Wang* and Pinhua Li*



8692

Crystalline covalent organic polymer as an effective zincophilic protective layer to boost the performance of aqueous zinc-ion batteries

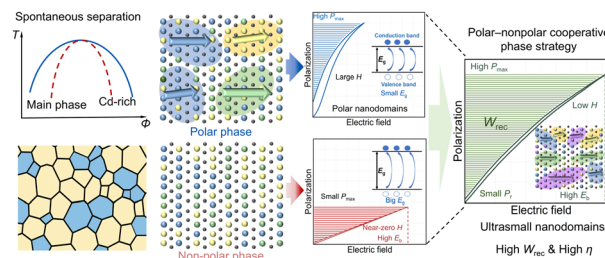
Xin Wang, Yuchan Zhang, Lei Zhang, Qianfeng Gu, Qi Liu, Yang Ren, Chun-Sing Lee* and Qichun Zhang*



8701

Hierarchical polar-nonpolar phase architecture enabling excellent lead-free capacitive energy storage

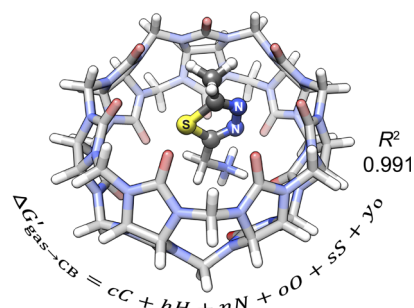
Qingqing Wu, Huajie Luo,* Yuhang Hu, Yuhui Huang, Xiangwei Guo,* Hubo Zhu, Haishan Xu, Shenglin Jiang, Tianyu Li* and Bing Xie*



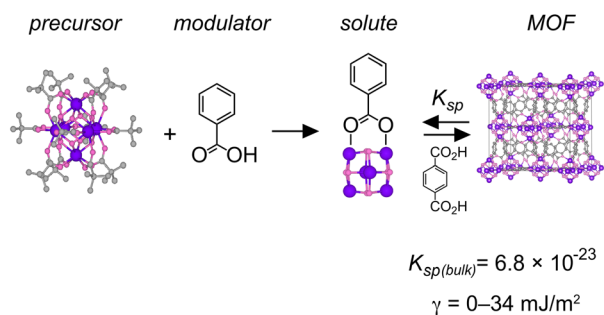
8712

Accurate prediction of cucurbituril binding affinities from guest molecular formulae

Josie Franks and Eric Masson*



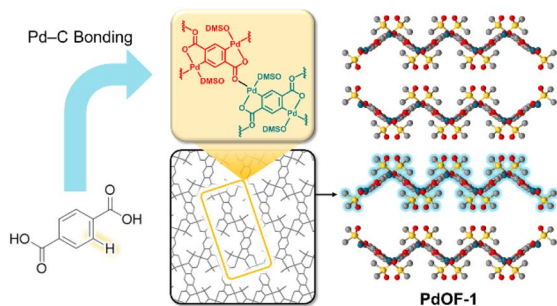
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Zr₆O₄(OH)₄(O₂C-*t*-Bu)₁₂ precursor uncovers how modulators govern supersaturation, nucleation, and growth of UiO-66 nanocrystals

Jade M. Kemp and Jonathan S. Owen*

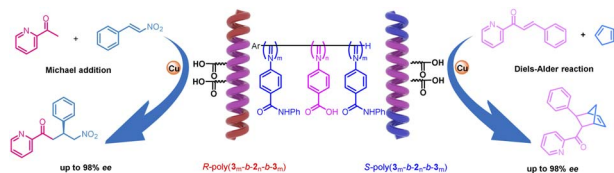
8726



Two-dimensional Pd-C bonded organometallic framework with dynamic packing transformations

Jong-Yeong Jung, Jaewook Kim, Jintaek Gong, Dongwook Kim, Hee-Seung Lee* and Hyunjoon Song*

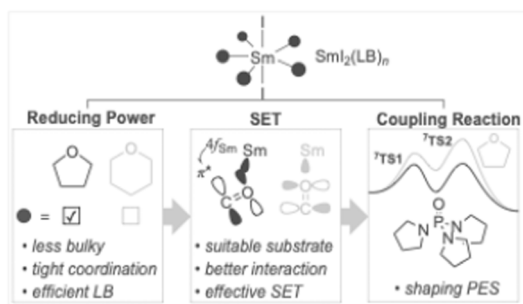
8733



Achiral benzoic acid appended helical polymers for the copper-catalyzed asymmetric Diels-Alder reaction and Michael addition with excellent enantioselectivity and recyclability

Qi-Hui Ti, Ming-Yang Mo, Run-Tan Gao, Na Liu* and Zong-Quan Wu*

8744



Computational study of the effect of Lewis base additives and molecular spin state in SmI₂-chemistry

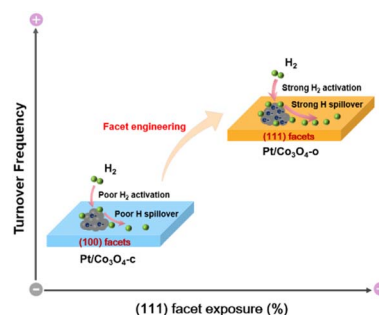
Song Yu, Ciro Romano, David J. Procter and Nikolas Kaltsoyannis*



8753

Promoted hydrogen activation and spillover over Pt/Co₃O₄ by facet engineering of Co₃O₄ for enhanced catalytic hydrogenation

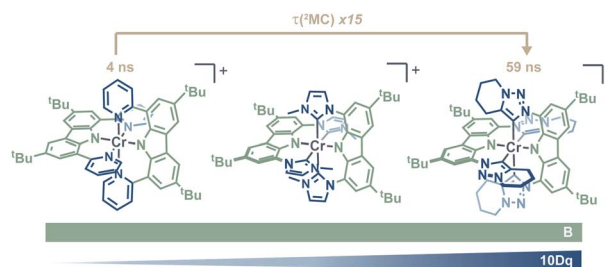
Hui Yun, Jiao Feng, Wanying Peng and Mi Xiong*



8760

Interplay between ligand field strength and the nephelauxetic effect in chromium(III) complexes with anionic amido ligands

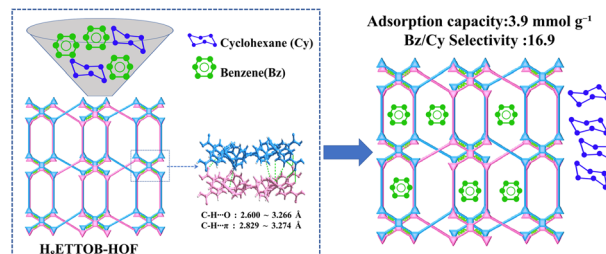
P. Yaltseva, B. Wittwer, D. Leitner, F. R. Neururer, F. Tambornino, A. Schmidt, D. Munz,* O. S. Wenger* and S. Hohloch*



8772

Rational design of a polyphenyl octacarboxylate HOF for highly selective separation of benzene over cyclohexane

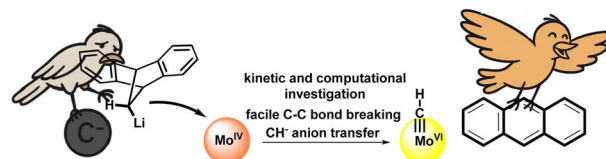
Biyang Liu, Ying Wang, Miao She, Tianfu Liu, Manxin Luo, Yongxin Xie, Defei Liu, Ziyi Du, Liyun Huang* and Wenbing Yuan*



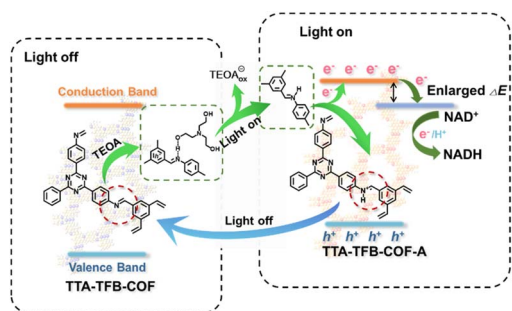
8780

A readily accessible CH anion transfer reagent for the preparation of a molybdenum methylidyne complex

Rajesh Mukkera, Nghia Le, Chandler I. Woo, Charles Edwin Webster* and Sidney E. Creutz*



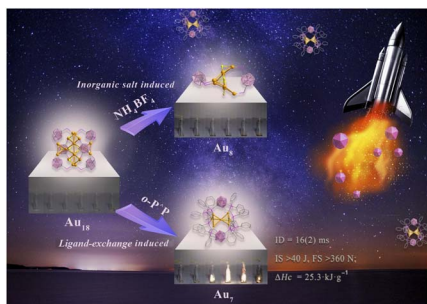
8787



Triethanolamine-activated imine-linked covalent organic frameworks for highly efficient NADH generation

Xiaoyu Li, Rui Liu, Han Cao, Chuanyin Tang, Guancheng Hua, Yingxu Hu, Xiangjiang Fan, Yongqing Xia and Shengjie Wang*

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Directing structural transformation in gold(i)-carborane nanoclusters to unlock ultrafast hypergolic ignition

Hao-Hui Xie, Wen-Jing Yang, Ze-Jian Li, Ying-Zheng Ren, Nian Si, Peng-Fei Liu, Yong-Xing Tang*, Wen-Chao Zhang* and Peng-Fei Cui*

CORRECTIONS

8803

Correction: Recent advances in MOF-based single-atom photocatalysts for CO₂ to solar fuel conversion under sunlight irradiation

Adnan Majeed, Minh-Khoa Duong, Van-Duc Nguyen and Trong-On Do*

8804

Correction: Theoretical insights into site-specific heavy-atom effects on MR-TADF emitters: modulation of spin-orbit coupling and color purity

Shi-Jie Ge, Jian-Rong Wu and Zuo-Quan Jiang*

