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Cover
See Katsuya Mutoh, Tatsuya Tsukuda, Takuya Nakashima *et al.*, pp. 8240–8246. Image reproduced by permission of Takuya Nakashima from *Chem. Sci.*, 2025, **16**, 8240.

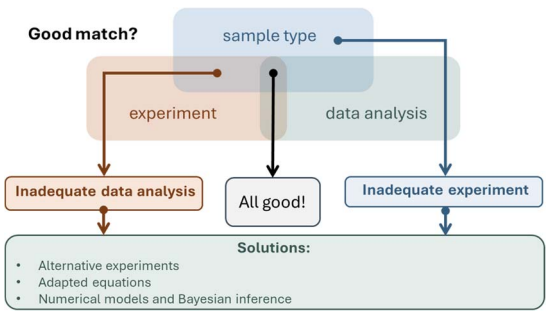
Inside cover
See Chris Ritchie *et al.*, pp. 8247–8261. Image reproduced by permission of Chris Ritchie from *Chem. Sci.*, 2025, **16**, 8247. Artist Credit - www.Sciencebrush.design.

PERSPECTIVES

8153

Challenges and opportunities for the characterization of electronic properties in halide perovskite solar cells

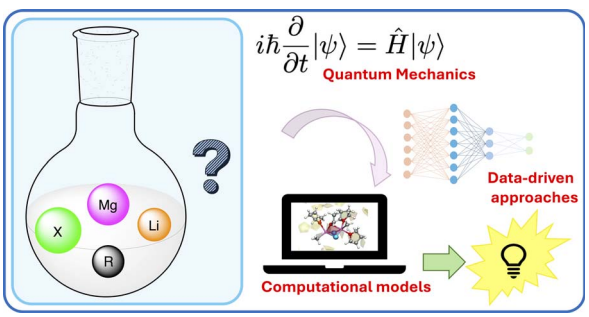
Thomas Kirchartz

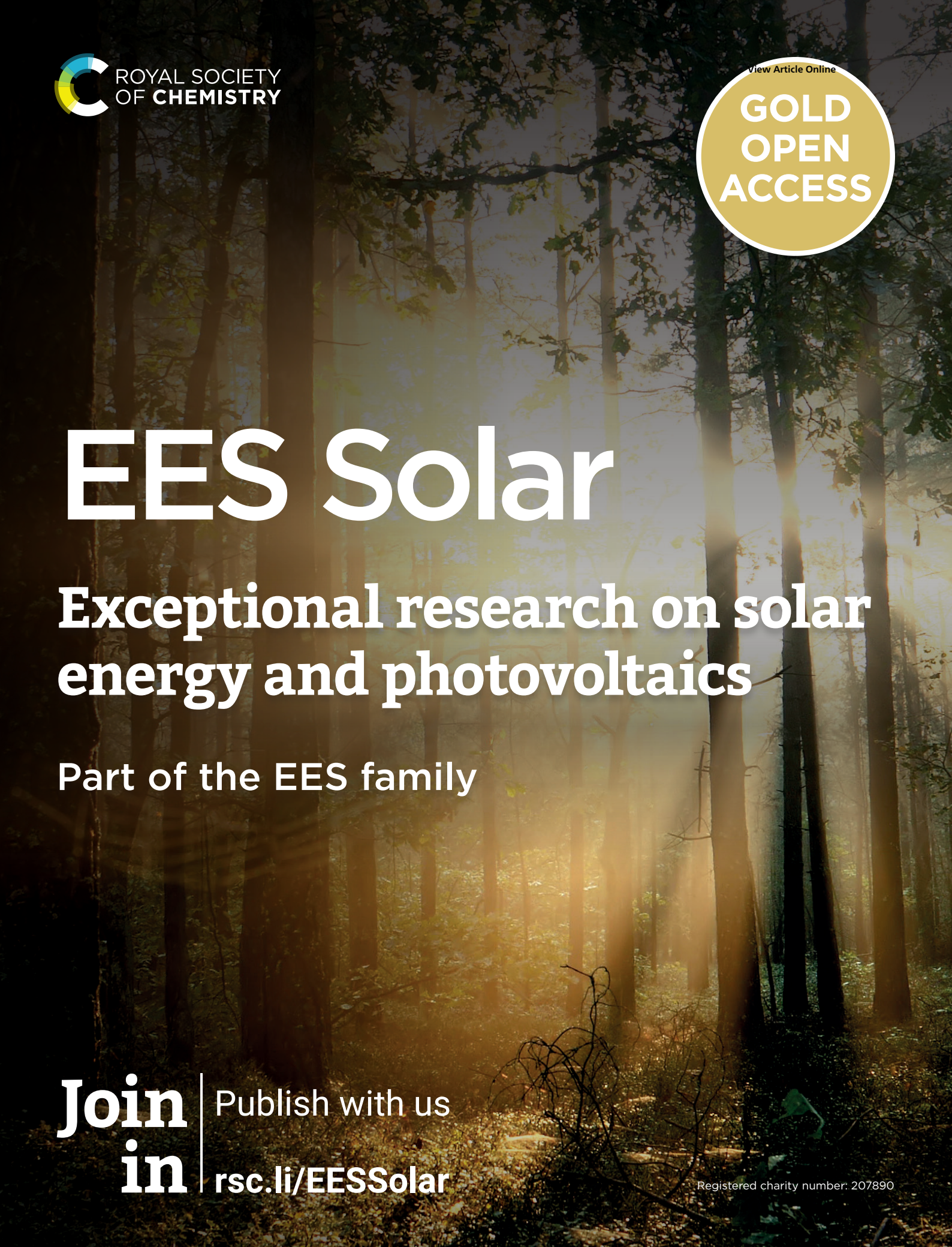


8196

The fellowship of the Grignard: 21st century computational tools for hundred-year-old chemistry

Michele Cascella,* Sigbjørn Løland Bore and Odile Eisenstein*

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REVIEW

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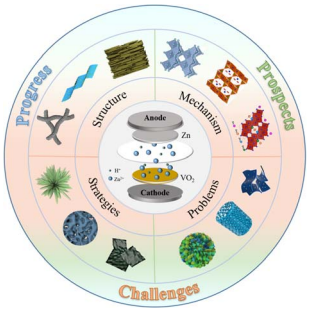
Critical issues and optimization strategies of vanadium dioxide-based cathodes towards high-performance aqueous Zn-ion batteries

Botao Wan, Yajiang Wang, Xiudong Chen,* Changchao Zhan, Huixiong Jiang, Jin-Hang Liu, Yun Gao,* Xiaoduo Jiang, Xiaohua Cao, Hang Zhang,* Shi-Xue Dou and Yao Xiao*

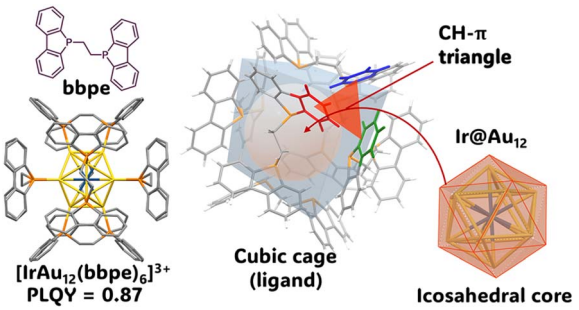


EDGE ARTICLES

8240

A nearly perfect icosahedral Ir@Au_{12} superatom with superior photoluminescence obtained by ligand engineering

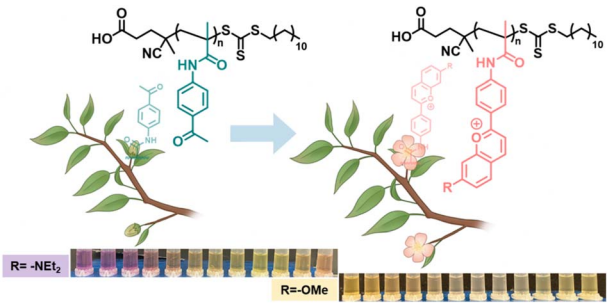
Katsuya Mutoh,* Teppei Yahagi, Shinjiro Takano, Sonomi Kawakita, Takeshi Iwasa, Tetsuya Taketsugu, Tatsuya Tsukuda* and Takuya Nakashima*



8247

Multi-stimuli-responsive polymers enabled by bio-inspired dynamic equilibria of flavylium chemistry

Yuxi Liu, Rico F. Tabor, Piotr Pawliszak, David A. Beattie, Marta Krasowska, Benjamin W. Muir, San H. Thang and Chris Ritchie*



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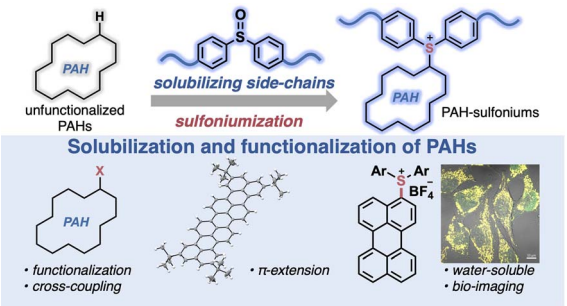
Functionalization and solubilization of polycyclic aromatic compounds by sulfoniumization

Johannes E. Erchinger, Tsubasa Okumura, Kanami Nakata, Daisuke Shimizu, Constanstin G. Daniliuc, Kazuma Amaike,* Frank Glorius, Kenichiro Itami* and Hideto Ito*



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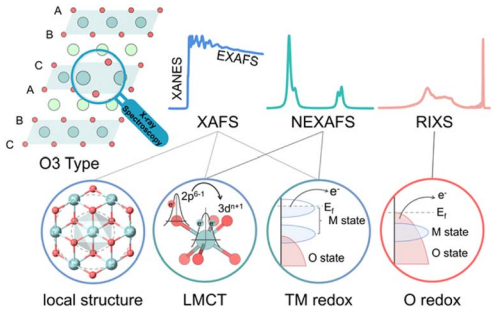
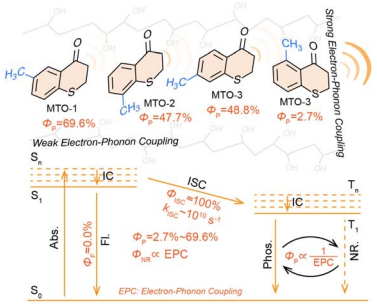


Reassessing anionic redox in conventional layered oxide cathodes for Li-ion batteries: ionic and covalent mechanisms

Jianhua Yin, Zixin Wu,* Kai Fang, Yuanlong Zhu, Kang Zhang, Haitang Zhang, Yilong Chen, Li Li, Longlong Fan, Kang Dong, Lirong Zheng, Qingsong Wang,* Huan Huang,* Jing Zhang,* Yu Qiao* and Shi-Gang Sun

8282



Manipulating room-temperature phosphorescence by electron–phonon coupling

Liangwei Ma, Muyu Cong, Siyu Sun and Xiang Ma*

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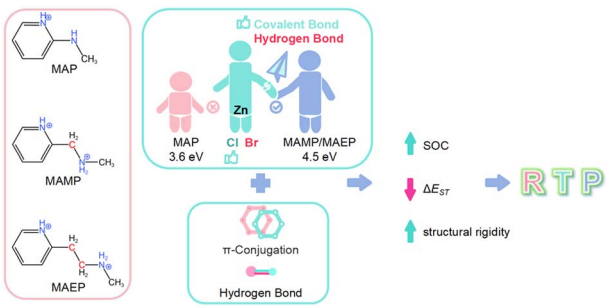

Tuning covalent bonding in zinc-based hybrid halides towards tunable room-temperature phosphorescence

Yibo Cui, Jiawei Lin, Kunjie Liu, Yuhe Shao, Dong Zhao, Zhongnan Guo, Jing Zhao,* Zhiguo Xia* and Quanlin Liu*

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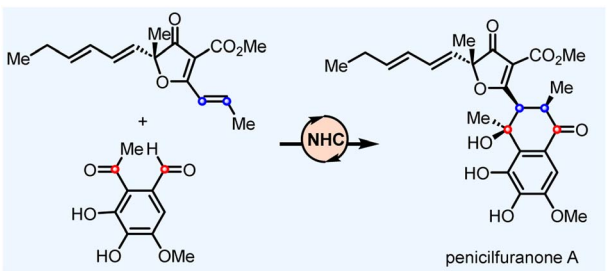


Asymmetric total synthesis of penicilfuranone A through an NHC-catalyzed umpolung strategy

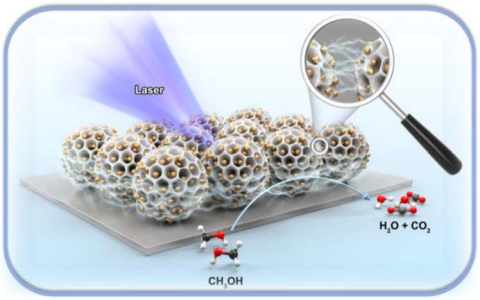
Yiming Ding, Xianwen Long, Jingwei Zhang, Chunlei Qu, Peng Wang, Xiaodong Yang, Pema-Tenzin Puno and Jun Deng*

EDGE ARTICLES

8309

Precise positioning of Au islands within mesoporous Pd–Pt nanoparticles for plasmon-enhanced methanol oxidation

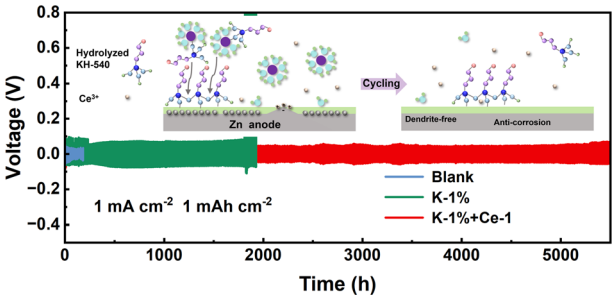
Liyang Zhu, Yunqing Kang, Miharu Eguchi,* Yingji Zhao, Dong Jiang, Xiaoqian Wei, Xingtao Xu, Kenta Nakagawa, Toru Asahi, Tokihiko Yokoshima* and Yusuke Yamauchi*



8319

Silane cooperation with $Ce_2(SO_4)_3$ to efficiently construct a protective layer and induce uniform deposition of Zn^{2+} for an ultra-stable Zn anode

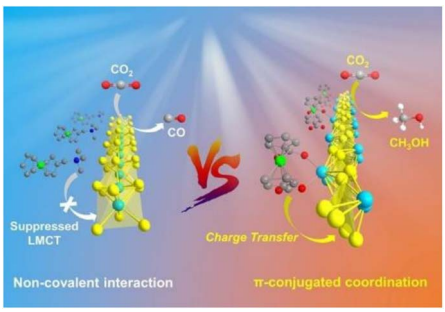
Luyan Yu, Sidan He, Baohua Liu, Mingrui Zhang, Houyi Ma, Chao Wang* and Qinghong Wang*



8327

Coordination-driven assembly of a ferrocene-functionalized lead iodide framework with enhanced stability and charge transfer for photocatalytic CO_2-to-CH_3OH conversion

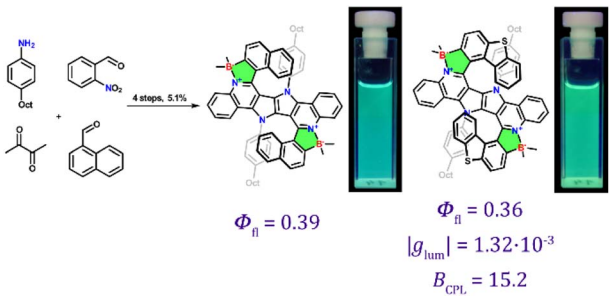
Jinlin Yin, Yani He, Chen Sun, Yilin Jiang and Honghan Fei*



8338

Double helicene possessing B–N dative bonds built on 1,4-dihydropyrrolo[3,2-*b*]pyrrole core

Wojciech D. Petrykowski, Nicolas Vanthuyne, Carmelo Naim, Francesco Bertocchi, Yevgen M. Poronik, Arkadiusz Ciesielski, Michał K. Cyrański,* Francesca Terenziani,* Denis Jacquemin* and Daniel T. Gryko*



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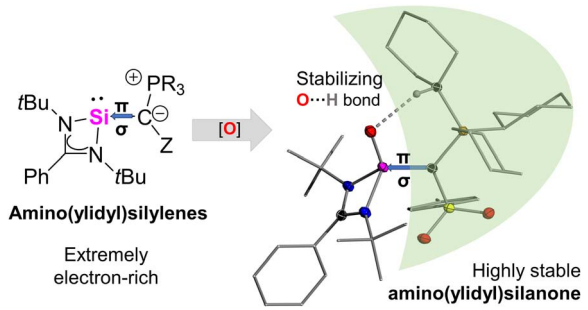
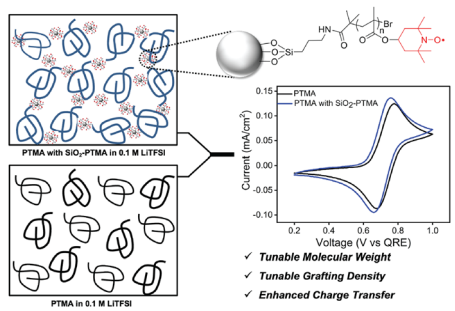


Base-stabilized acyclic amino(ylidyl)silylenes: electron-rich donors for the stabilization of silicon-element multiple bonds

Felix Krischer, Stephan Mayer, Lennart Hensle, Daniel Knyszek, Heidar Darmandeh and Viktoria H. Gessner*

8357



Redox-active polymer-grafted particles as redox mediators for enhanced charge transport in solution-state electrochemical systems

Mohd Avais, Ratul Mitra Thakur, Evan Fox, Jodie L. Lutkenhaus* and Emily B. Pentzer*

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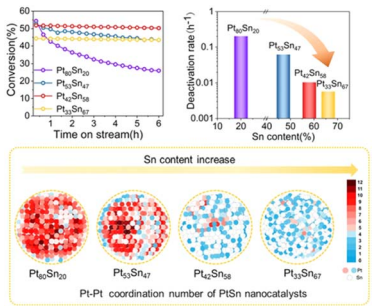
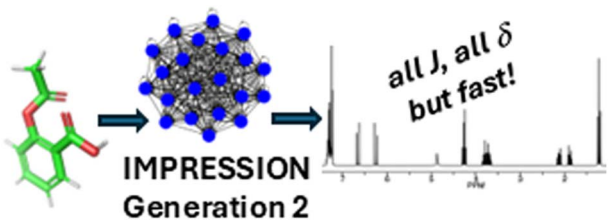


Atomic surface structure for unraveling the trade-off between the propane dehydrogenation activity and anti-deactivation of PtSn catalysts

Mingxin Lv, Qiang Li,* Fan Xue, Zhiguo Li, Peixi Zhang, Yue Zhu, Longlong Fan, Jianrong Zeng, Qiheng Li, Xin Chen, Kun Lin, Jinxia Deng and Xianran Xing*

8377



IMPRESSION generation 2 – accurate, fast and generalised neural network model for predicting NMR parameters in place of DFT.

Calvin Yiu, Ben Honoré, Will Gerrard, Jose Napolitano-Farina, Dave Russell, Iuni Margaret Laura Trist, Ruth Dooley and Craig P. Butts*

EDGE ARTICLES

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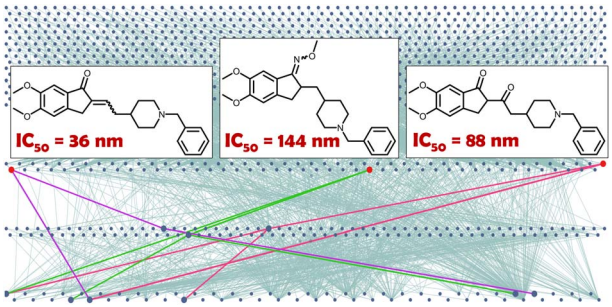
Retro-forward synthesis design and experimental validation of potent structural analogs of known drugs

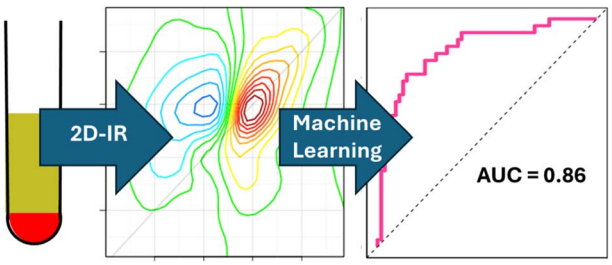
Ahmad Makkawi, Wiktor Beker, Agnieszka Wołos, Sabyasachi Manna, Rafał Roszak, Sara Szymkuć, Martyna Moskal, Aleksei Koshevarnikov, Karol Molga, Anna Żądło-Dobrowolska* and Bartosz A. Grzybowski*



8394

Machine-learning based classification of 2D-IR liquid biopsies enables stratification of melanoma relapse risk

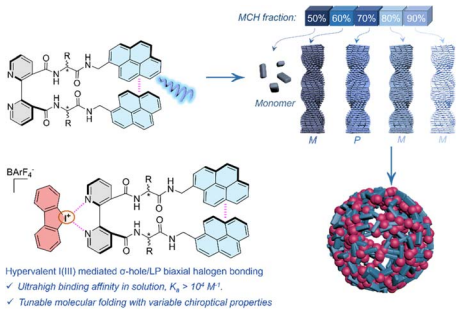
Kelly Brown, Amy Farmer, Sabina Gurung, Matthew J. Baker, Ruth Board and Neil T. Hunt*



8405

Hierarchical chirality conversion switched by biaxial halogen bonding

Weilong Ma, Zhaozhen Cao, Na Zhang,* Aiyou Hao and Pengyao Xing*



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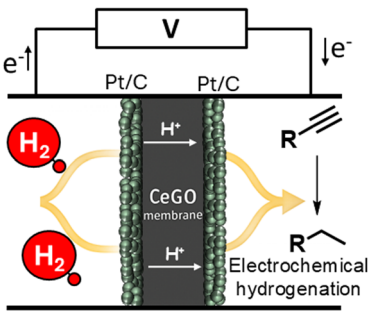
Electrocatalytic hydrogenation of alkynes and alkenes using a proton conductive graphene oxide membrane

Muhammad Sohail Ahmad, Imam Sahroni, Taiga Kodama, Kazuto Hatakeyama and Tetsuya Kida*



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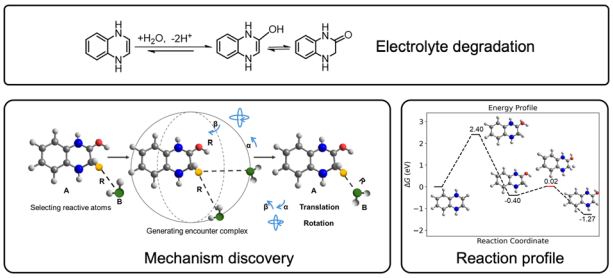
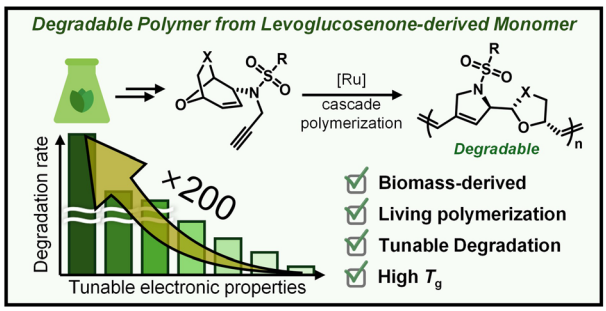


Computational framework for discovery of degradation mechanisms of organic flow battery electrolytes

Xiaotong Zhang and Piotr de Silva*

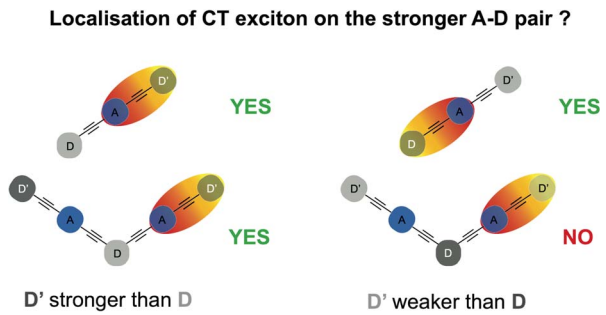
8435



Controlled polymerization of levoglucosenone-derived enynes to give bio-based polymers with tunable degradation rates and high glass transition temperatures

Eunsong Jung, Antonio Rizzo, Hanseul Ryu, Minyoung Cho and Tae-Lim Choi*

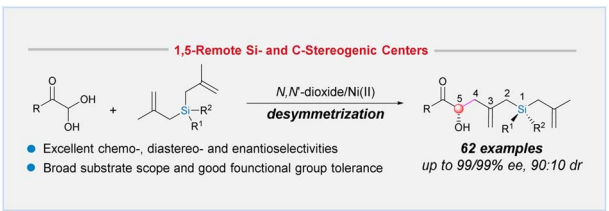
8443



Controlling the spatial distribution of electronic excitation in asymmetric D–A–D′ and symmetric D′–A–D–A–D′ electron donor–acceptor molecules

Evangelos Balanikas, Tommaso Bianconi, Pietro Mancini, Nikhil Ji Tiwari, Manju Sheokand, Rajneesh Misra,* Benedetta Carlotti* and Eric Vauthey*

8454



Catalytic asymmetric construction of 1,5-remote Si- and C-stereocenters *via* desymmetrizing ene reaction of bis(methallyl)silanes

Qiuhui Cao, Yuntian Yang, Yiwen Mei, Minghui Ji, Fei Wang, Xiaoming Feng* and Weidi Cao*

EDGE ARTICLES

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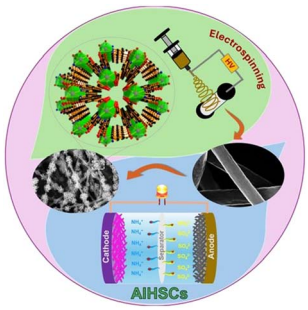
Tailored design of an oxygen-rich stable Co-MOF integrated with MXene nanofibers as an advanced heterostructure for high-performance ammonium-ion supercapacitors

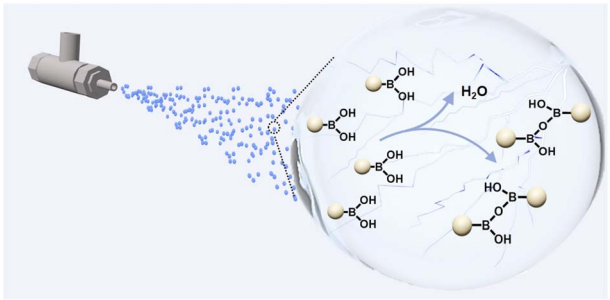
Nissar Hussain and Shaikh M. Mobin*



8470

Electric-field-induced covalent condensation of boronic acids in water microdroplets

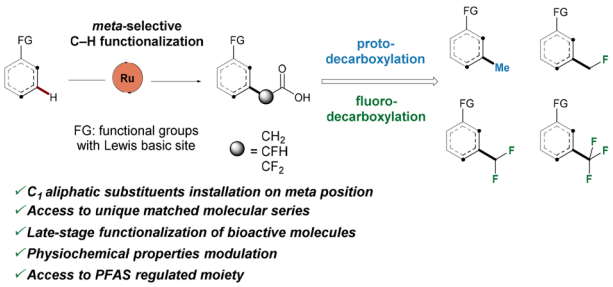
Yue-Wen Zhou, Ming-Yang Jia, Jun-Lei Yang, Qinlei Liu* and Zhen-Feng Cai*



8478

A unified approach to *meta*-selective methylation, mono-, di- and trifluoromethylation of arenes

Elisa Y. Lai, Lutz Ackermann* and Magnus J. Johansson*



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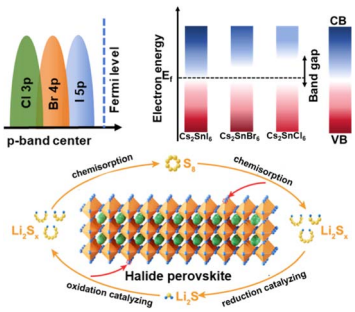
Insights into the halogen-induced p-band center regulation promising high-performance lithium–sulfur batteries

Hanzhang Fang, Wenshuo Hou,* Chuanlong Li, Shuo Li, Fulu Chu, Xuting Li, Xianping Zhang,* Linrui Hou, Changzhou Yuan* and Yanwei Ma



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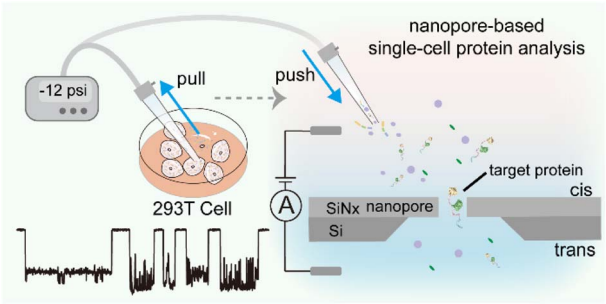
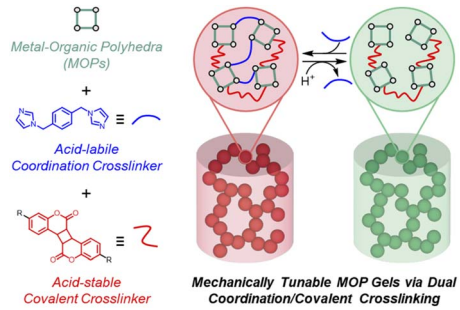


Exploring a solid-state nanopore approach for single-molecule protein detection from single cells

Zi-Qi Zhou, Shao-Chuang Liu,* Jia Wang, Ke-Le Chen, Bao-Kang Xie, Yi-Lun Ying and Yi-Tao Long*

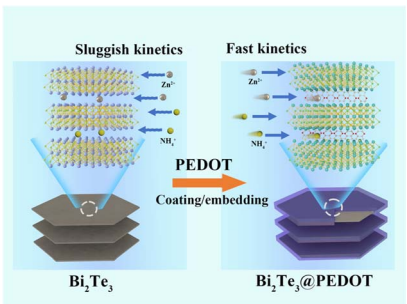
8509



Mechanically tunable porous gels constructed *via* the dual coordination/covalent polymerization of coumarin-functionalized rhodium–organic cuboctahedra

David W. Burke,* Masataka Yamashita, Zaoming Wang, Mako Kuzumoto, Kenji Urayama, Kei Saito and Shuhei Furukawa*

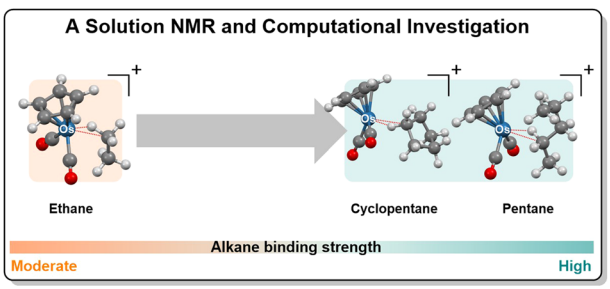
8523



Interlayer engineering-induced charge redistribution in Bi_2Te_3 toward efficient Zn^{2+} and NH_4^+ storage

Xiaojie Liang, Fangzhong Liu, Haonan Yue, Yaoyong Dong, Lijuan Chen, Ting Song, Yong Pei, Xianyou Wang, Bei Long,* Yao Xiao* and Xiongwei Wu*

8532



Coordination of ethane, pentane and cyclopentane to a cationic osmium complex: comparisons in alkane binding

James D. Watson, Dejan Mizdrak, Leslie D. Field* and Graham E. Ball*

EDGE ARTICLES

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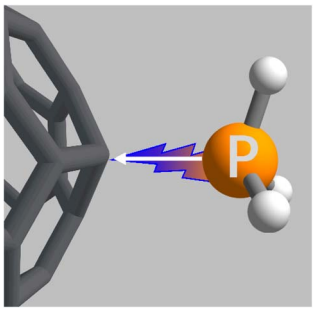
External electric fields drive the formation of P → C dative bonds

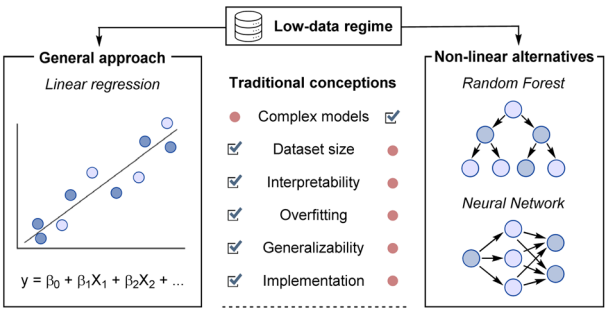
Tingting Ma, Xubin Wang, Xinru Peng, Jiayao Li, Shiwei Yin, Yirong Mo* and Changwei Wang*



8555

Machine learning workflows beyond linear models in low-data regimes

David Dalmau, Matthew S. Sigman and Juan V. Alegre-Requena*



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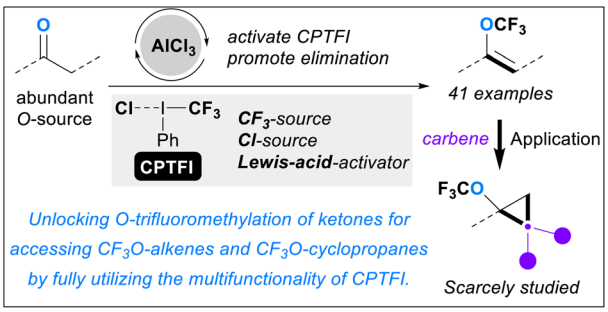
***O*-Trifluoromethylation of ketones: an alternative straightforward route to alkenyl trifluoromethyl ethers**

Chi Gao, Yang Liu, Cheng-Sheng Li, He Guo, Sheng-Han Wang, Cong Xu* and Mang Wang*



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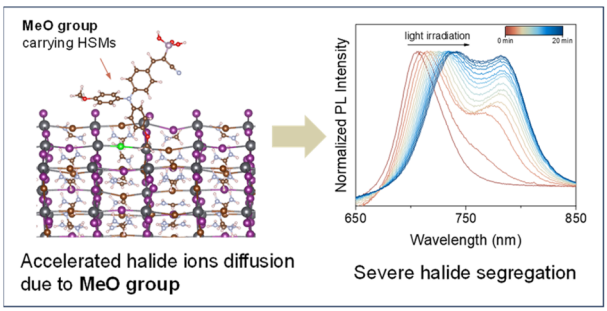
Correlating halide segregation of wide-bandgap perovskites with the methoxy group in organic hole-selective materials

Xiaoyu Ji, Yun Zhao, Xiaofeng Chen, Shuo Zhang,* Liqing Zhan, Huidong Zhang, Weizhong Zheng, Wei-Hong Zhu and Yongzhen Wu*



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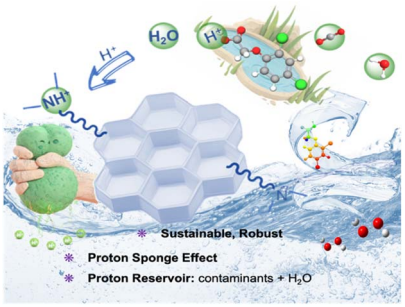

Harmonizing proton sponge and proton reservoir in conjugated microporous polymers for enhanced photocatalytic hydrogen peroxide production

Shiyuan Zhou, Wenwen Chen, Xiaobo Luo, Wenxiu Guo, Jingwen Dong, Yuxi Liu, Yuzhe Zhang, Danfeng Wang,* Zhongyu Li* and Peiyang Gu*

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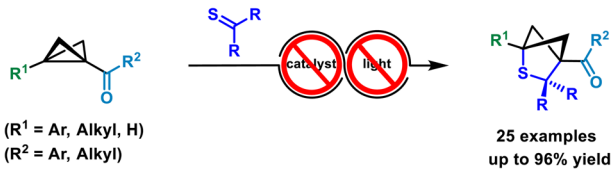

(3 + 2)-Cycloaddition of bicyclobutanes and thioketones: access to 2-thiabicyclo[2.1.1]hexanes without the use of catalysts or light

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