

Chemical Science

rsc.li/chemical-science

The Royal Society of Chemistry is the world's leading chemistry community. Through our high impact journals and publications we connect the world with the chemical sciences and invest the profits back into the chemistry community.

IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(3) 783–1164 (2024)



Cover
See Yasutaka Kuwahara, Hiromi Yamashita *et al.*, pp. 854–878. Image reproduced by permission of Yasutaka Kuwahara from *Chem. Sci.*, 2024, 15, 854.



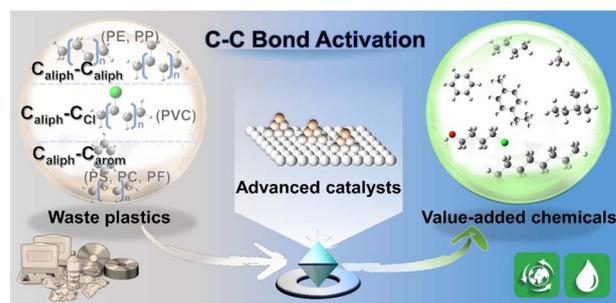
Inside cover
See Yu Wang *et al.*, pp. 896–905. Image reproduced by permission of Yu Wang from *Chem. Sci.*, 2024, 15, 896.

PERSPECTIVES

795

Precise activation of C–C bonds for recycling and upcycling of plastics

Hongshun Ran, Shuo Zhang, Wenyi Ni and Yaxuan Jing*



832

The thermodynamics and kinetics of depolymerization: what makes vinyl monomer regeneration feasible?

Victoria Lohmann, Glen R. Jones, Nghia P. Truong and Athina Anastasaki*



EES Catalysis

GOLD
OPEN
ACCESS

Exceptional research on energy
and environmental catalysis

Open to everyone. Impactful for all

rsc.li/EESCatalysis

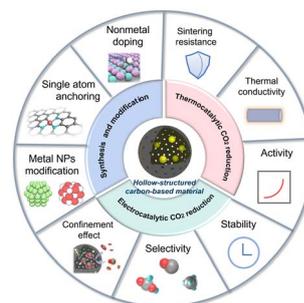
Fundamental questions
Elemental answers

REVIEWS

854

Hollow carbon-based materials for electrocatalytic and thermocatalytic CO₂ conversion

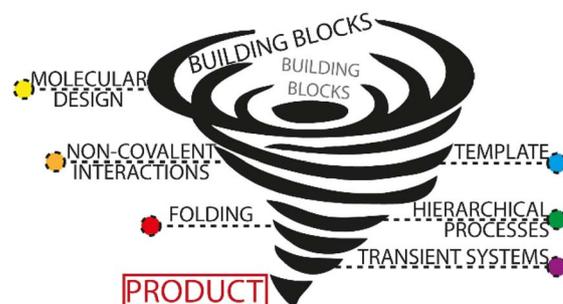
Kaining Li, Yasutaka Kuwahara* and Hiromi Yamashita*



879

Dynamic covalent synthesis

Fabien B. L. Cougnon,* Artur R. Stefankiewicz* and Sébastien Ulrich*

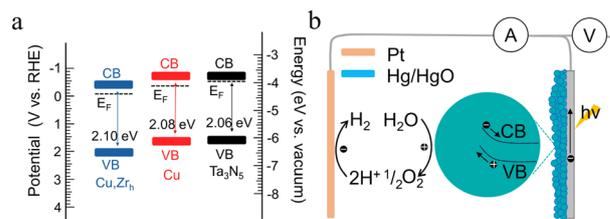


EDGE ARTICLES

896

Engineering band structuring via dual atom modification for an efficient photoanode

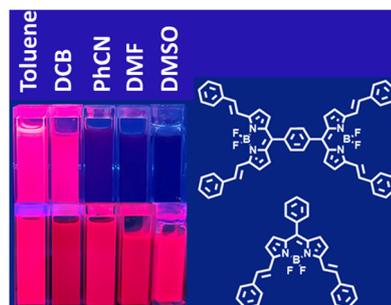
Xiaodong Wang, Huijuan Zhang, Chuanzhen Feng and Yu Wang*



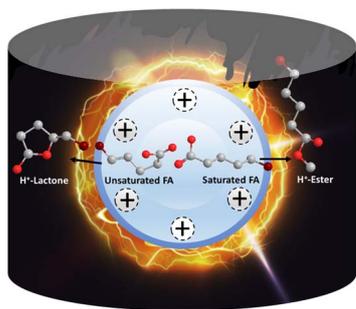
906

Symmetry breaking charge transfer leading to charge separation in a far-red absorbing bisstyryl-BODIPY dimer

Aida Yahagh, Ram R. Kaswan, Shahrzad Kazemi, Paul A. Karr and Francis D'Souza*



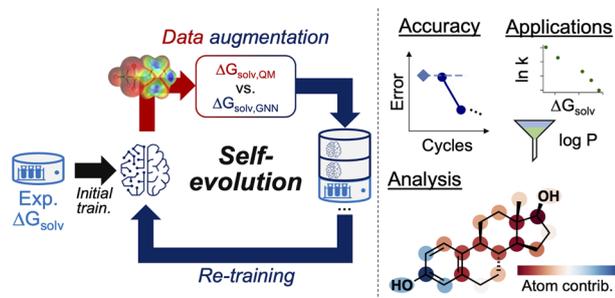
914



Charge inversion under plasma-nanodroplet reaction conditions excludes Fischer esterification for unsaturated fatty acids: a chemical approach for type II isobaric overlap

Dmytro S. Kulyk, Glib V. Baryshnikov, Purva S. Damale, Simon Maher and Abraham K. Badu-Tawiah*

923



Designing solvent systems using self-evolving solubility databases and graph neural networks

Yeonjoon Kim, Hojin Jung, Sabari Kumar, Robert S. Paton and Seonah Kim*

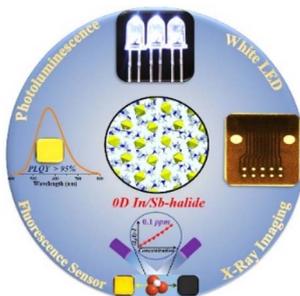
940



Suppressing ACQ of molecular photosensitizers by distorting the conjugated-plane for enhanced tumor photodynamic therapy

Han Sun, Lukun Li, Ruihua Guo, Zhe Wang,* Yanhui Guo, Zhiliang Li* and Fengling Song*

953



A 0D hybrid lead-free halide with near-unity photoluminescence quantum yield toward multifunctional optoelectronic applications

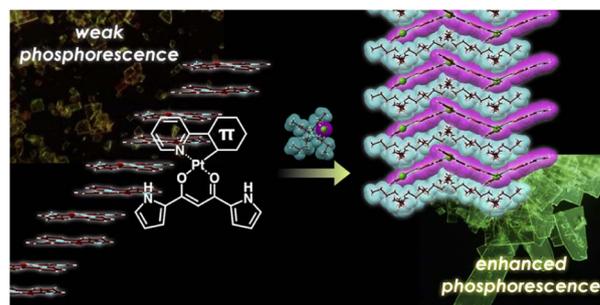
Dong-Yang Li, Huai-Yuan Kang, Yu-Hang Liu, Jie Zhang, Cheng-Yang Yue, Dongpeng Yan* and Xiao-Wu Lei*



964

Enhanced solid-state phosphorescence of organoplatinum π -systems by ion-pairing assembly

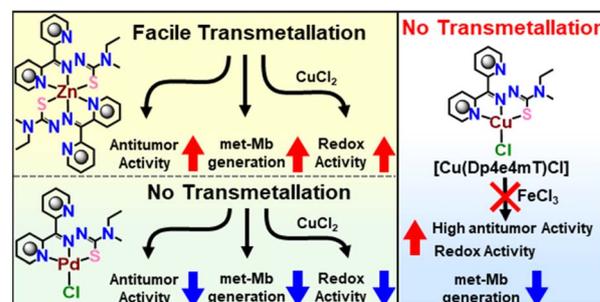
Yohei Haketa, Kaifu Komatsu, Hiroi Sei, Hiroki Imoba, Wataru Ota, Tohru Sato, Yu Murakami, Hiroki Tanaka, Nobuhiro Yasuda, Norimitsu Tohnai and Hiromitsu Maeda*



974

Differential transmetalation of complexes of the anti-cancer thiosemicarbazone, Dp4e4mT: effects on anti-proliferative efficacy, redox activity, oxy-myoglobin and oxy-hemoglobin oxidation

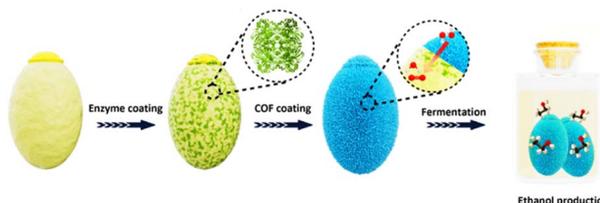
Mahendiran Dharmasivam,* Busra Kaya, Tharushi P. Wijesinghe, Vera Richardson, Jeffrey R. Harmer, Miguel A. Gonzalez, William Lewis, Mahan Gholam Azad, Paul V. Bernhardt and Des R. Richardson*



991

Covalent-organic framework nanobionics for robust cytoprotection

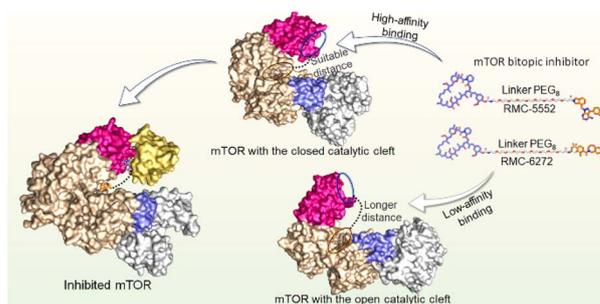
Jieying Liang,* Qianfan Chen, Joel Yong, Hiroki Suyama, Joanna Biazik, Bosiljka Njegic, Aditya Rawal and Kang Liang*



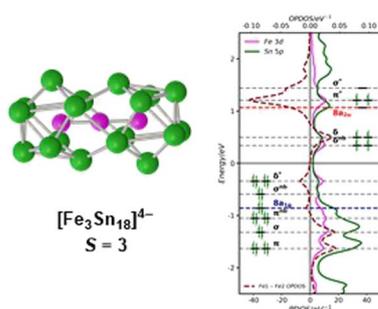
1003

The allosteric mechanism of mTOR activation can inform bitopic inhibitor optimization

Yonglan Liu, Mingzhen Zhang, Hyunbum Jang and Ruth Nussinov*



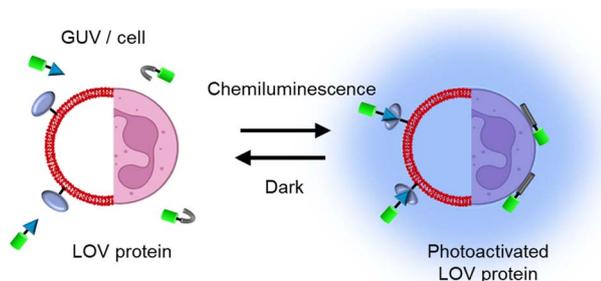
1018



Snap-shots of cluster growth: structure and properties of a Zintl ion with an Fe₃ core, [Fe₃Sn₁₈]⁴⁻

Zi-Sheng Li, Wei-Xing Chen, Harry W. T. Morgan, Cong-Cong Shu, John E. McGrady* and Zhong-Ming Sun*

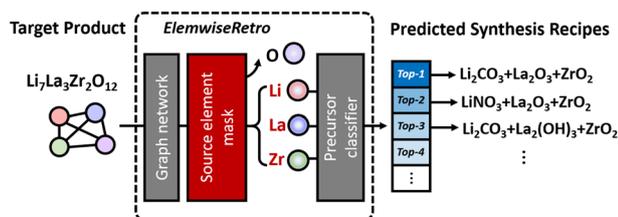
1027



Photoactivation of LOV domains with chemiluminescence

Yuhao Ji, Ali Heidari, Brice Nzigou Mombo and Seraphine V. Wegner*

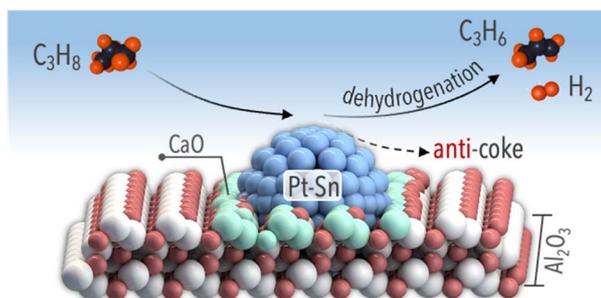
1039



Predicting synthesis recipes of inorganic crystal materials using elementwise template formulation

Seongmin Kim, Juhwan Noh, Geun Ho Gu, Shuan Chen and Yousung Jung*

1046



Alkaline-earth ion stabilized sub-nano-platinum tin clusters for propane dehydrogenation

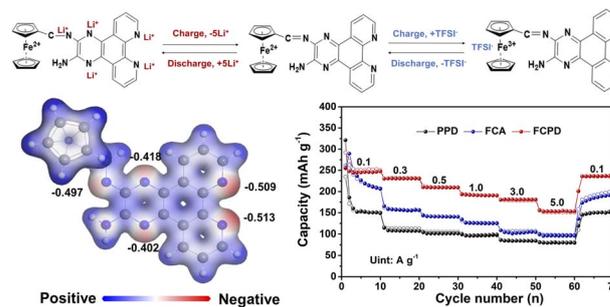
Zhenpu Lu, Ran Luo, Sai Chen, Donglong Fu, Guodong Sun, Zhi-Jian Zhao, Chunlei Pei* and Jinlong Gong*



1051

Design of a bipolar organic small-molecule cathode with mesoporous nanospheres structure for long lifespan and high-rate Li-storage performance

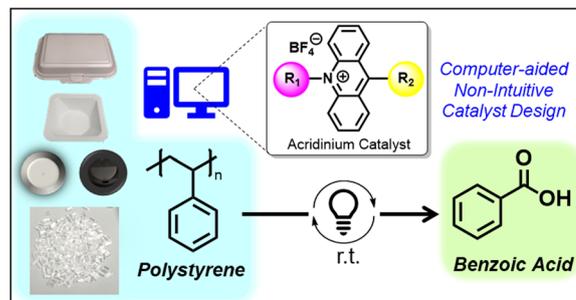
Simin Wang, Qifei Guo, Haoran Liu, Longhai Zhang, Chaofeng Zhang, Tengfei Zhou, Quanwei Ma, Hongbao Li,* Rui Wang and Yang Zheng*



1061

Enhancing the photocatalytic upcycling of polystyrene to benzoic acid: a combined computational-experimental approach for acridinium catalyst design

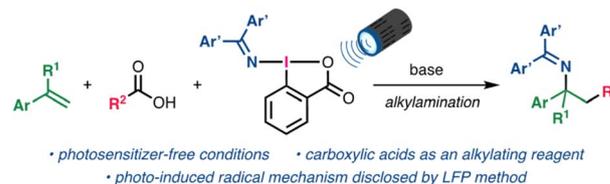
Albert Ong, Zi Cheng Wong, Kang Le Osmund Chin, Wei Wei Loh, Ming Hui Chua,* Shi Jun Ang* and Jason Y. C. Lim*



1068

Photoexcitation of (diarylmethylene)amino benziodoxolones for alkylation of styrene derivatives with carboxylic acids

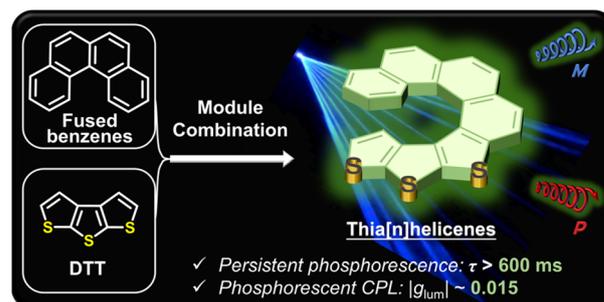
Daichi Okumatsu, Kensuke Kiyokawa,* Linh Tran Bao Nguyen, Manabu Abe* and Satoshi Minakata*



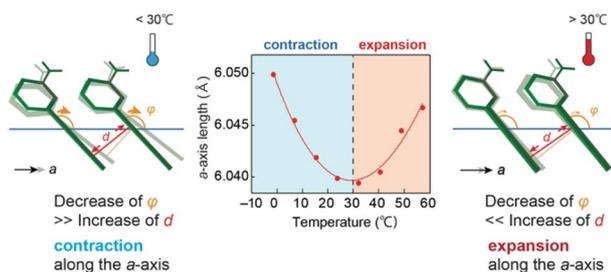
1077

Thia[n]helicenes with long persistent phosphorescence

Zhen Sun, Wan Xu, Shuai Qiu, Zhiying Ma, Chunli Li, Sheng Zhang* and Hua Wang*



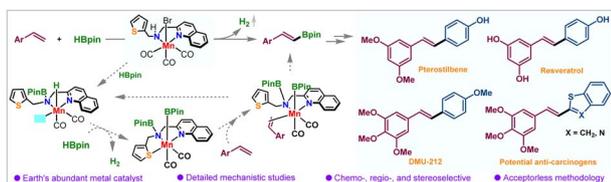
1088



Negative to positive axial thermal expansion switching of an organic crystal: contribution to multistep photoactuation

Shodai Hasebe, Yuki Hagiwara, Takashi Ueno, Toru Asahi and Hideko Koshima*

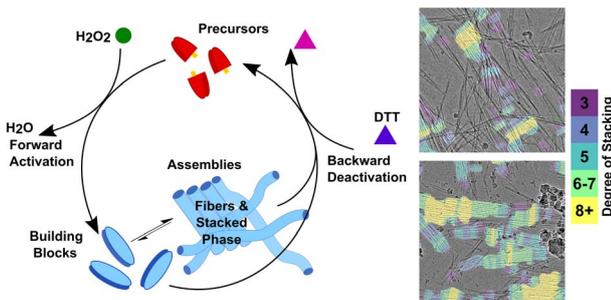
1098



Catalytic acceptorless dehydrogenative borylation of styrenes enabled by a molecularly defined manganese complex

Kuhali Das, Abhishek Kundu, Koushik Sarkar, Debashis Adhikari* and Biplab Maji*

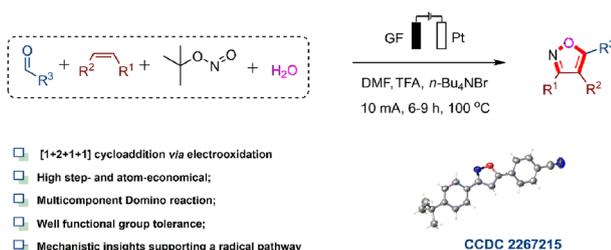
1106



CryoEM reveals the complex self-assembly of a chemically driven disulfide hydrogel

Paul Joshua Hurst, Justin T. Mulvey, Rebecca A. Bone, Serxho Selmani, Redford F. Hudson, Zhibin Guan, Jason R. Green and Joseph P. Patterson*

1117



Electrochemical assembly of isoxazoles via a four-component domino reaction

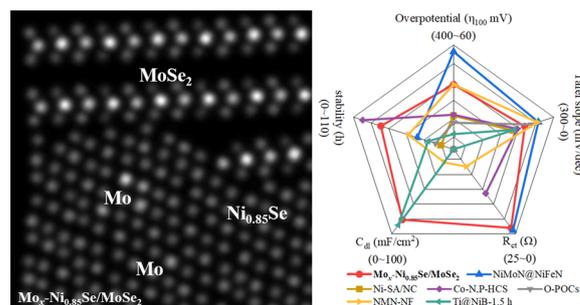
Yuanyuan Zhao, Xinyue Li, Simon L. Homölle, Bin Wang* and Lutz Ackermann*



1123

Mo-doping heterojunction: interfacial engineering in an efficient electrocatalyst for superior simulated seawater hydrogen evolution

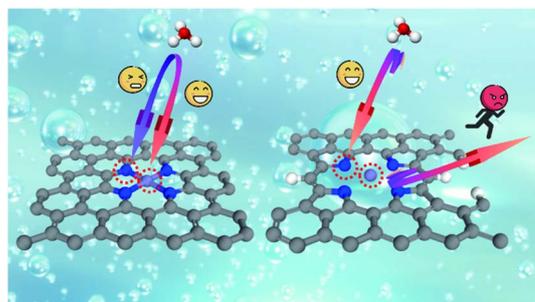
Zuo-Ming He, Chun-Xiao Zhang, Si-Qi Guo, Peng Xu, Yuan Ji, Si-Wei Luo, Xiang Qi, Yun-Dan Liu,* Ning-Yan Cheng,* Shi-Xue Dou, Yun-Xiao Wang* and Bin-Wei Zhang*



1132

The role of nitrogen sources and hydrogen adsorption on the dynamic stability of Fe–N–C catalysts in oxygen reduction reaction

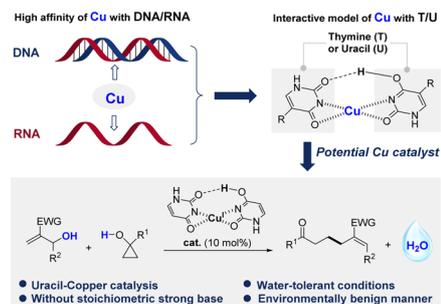
Zhou Huang, Fuhua Li, Yongduo Liu, Siguo Chen, Zidong Wei* and Qing Tang*



1143

Uracil-Cu(I) catalyst: allylation of cyclopropanols with Morita–Baylis–Hillman alcohols under water-tolerant conditions

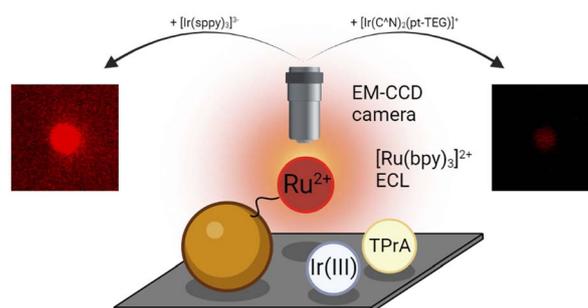
Jingwei Hou, Xiaohong Li, Kaiyu Yan, Lei Zhang,* Teck-Peng Loh* and Peizhong Xie*



1150

Redox-mediated electrochemiluminescence enhancement for bead-based immunoassay

Alessandro Fracassa, Claudio Ignazio Santo, Emily Kerr, Sara Knežević, David J. Hayne, Paul S. Francis, Frederic Kanoufi, Neso Sojic, Francesco Paolucci and Giovanni Valentini*



CORRECTIONS

1159

Correction: When SF₅ outplays CF₃: effects of pentafluorosulfanyl decorated scorpionates on copper

Anurag Noonikara-Poyil, Alvaro Muñoz-Castro, Andrii Boretskyi, Pavel K. Mykhailiuk* and H. V. Rasika Dias*

1162

Correction: Synthetic ramoplanin analogues are accessible by effective incorporation of arylglycines in solid-phase peptide synthesis

Edward Marschall, Rachel W. Cass, Komal M. Prasad, James D. Swarbrick, Alasdair I. McKay, Jennifer A. E. Payne, Max J. Cryle* and Julien Tailhades*

