Open Access Article. Published on 01 October 2025. Downloaded on 12/29/2025 8:38:05 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

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 16(38) 17509–17972 (2025)

Cover
See Véronique Michelet *et al.*, pp. 17611–17620. Image reproduced by permission of Emilie Gentilini and Véronique Michelet from *Chem. Sci.*, 2025, **16**, 17611.
The authors wish to acknowledge Université Côte d'Azur & Institut Servier d'Innovation Thérapeutique Paris-Saclay.

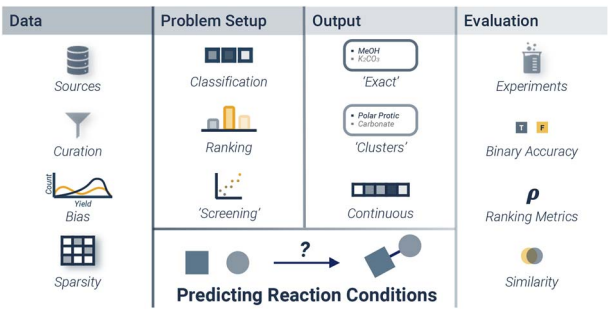
Inside cover
See Ryusei Oketani, Ichiro Hisaki *et al.*, pp. 17621–17629. Image reproduced by permission of Musashi Okada and Ryusei Oketani from *Chem. Sci.*, 2025, **16**, 17621.

PERSPECTIVES

17523

Predicting reaction conditions: a data-driven perspective

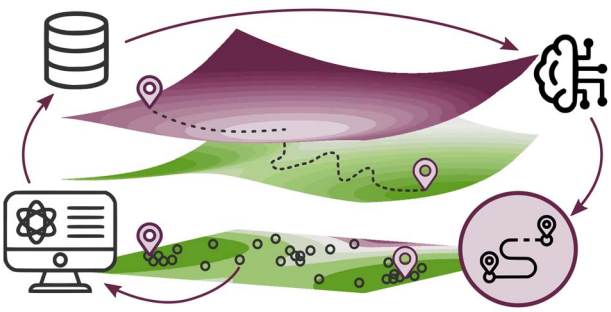
Matthew Ball, Dragos Horvath, Thierry Kogej, Mikhail Kabeshov and Alexandre Varnek*



17542

Machine learning for nonadiabatic molecular dynamics: best practices and recent progress

Carolin Müller, Štěpán Sršeň, Brigitta Bachmair, Rachel Crespo-Otero, Jingbai Li, Sascha Mausenberger, Max Pinheiro, Jr, Graham Worth, Steven A. Lopez* and Julia Westermayr*



ROYAL SOCIETY OF CHEMISTRY

View Article Online

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

Registered charity number: 207890

Open Access Article. Published on 01 October 2025. Downloaded on 12/29/2025 8:38:05 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

REVIEWS

17568

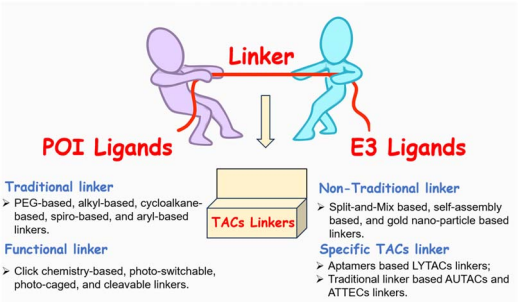
Single-atom catalysts meet electrospinning: a blissful marriage for energy catalysis

Bingyan Shi and Xiaofeng Lu*

17595

Rational design of the linkers in targeting chimeras

Yiping Duan, Michelle Y. Cai, Jinyi Xu* and Quanyin Hu*

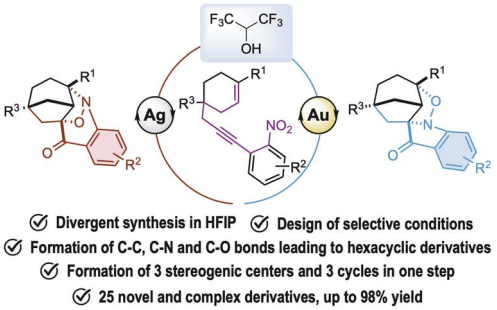


EDGE ARTICLES

17611

Silver- and gold-catalyzed divergent cascade cycloisomerization/[3 + 2] *versus* [2 + 2 + 1] cycloaddition towards a stereoselective access to heterohexacyclic derivatives

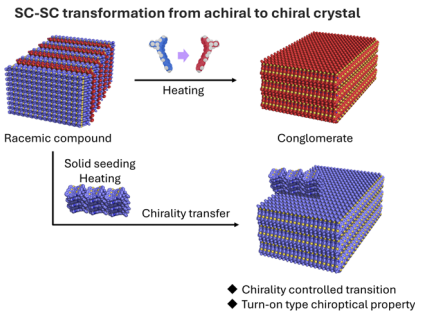
Emilie Gentilini, Anaïs Bouschon, Vincent Davenel, Fabien Fontaine-Vive, Jean-Marie Fourquez and Véronique Michelet*



17621

Spontaneous chiral symmetry breaking in a single crystal

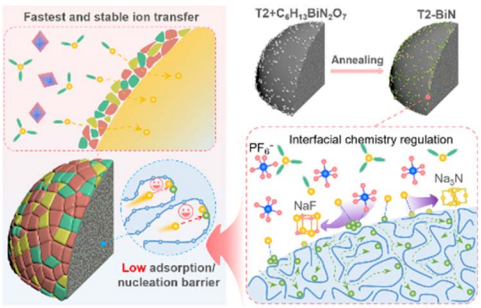
Ryusei Oketani,* Musashi Okada, Kentaro Takaji, Hajime Shigemitsu, Toshiyuki Kida, Takuya Nakashima and Ichiro Hisaki*



Open Access Article. Published on 01 October 2025. Downloaded on 12/29/2025 8:38:05 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

EDGE ARTICLES

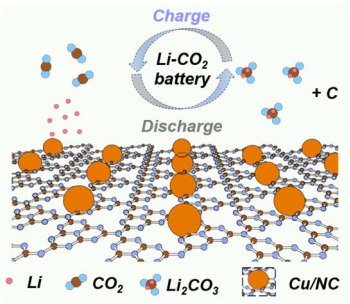
17630



Interfacial chemistry regulation by orbital hybridization for superior kinetics of hard carbon in an ester-based electrolyte

Lu Liu, Jianhua Zhu, Guohui Chen, Zhuosen Wang, Liu Wang, Chengkun Guo, Yunfeng Chao,* Xinwei Cui* and Caiyun Wang

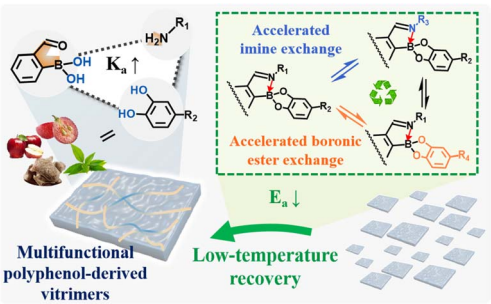
17640



Synergistic Cu-based catalysts with multiple active sites for high-efficiency Li–CO_2 batteries

Shasha Xiao, Ying Xiao,* Gang He, Tonghui Zhang, Longlong Yang, Feng Huo and Shimou Chen*

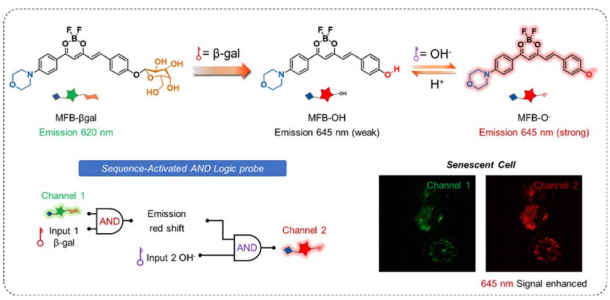
17649



Iminoboronate chemistry enables multifunctional and reprocessable polyphenol-derived vitrimers

Zhan Li, Bo Liang, Rong Zhang, Lei Yang, Xiancheng Ren, Shaohui Xiong, Wei Zhang, Junfei Hu,* Zhipeng Gu* and Yiwen Li*

17658



A sequence-activated near-infrared fluorescence probe for precisely tracking *in vivo* senescence

Jiahuan Nong, Pengcheng Li, Mingming Zhu,* Yifeng Li, Changsheng Wang, Yutao Zhang, Chenxu Yan and Zhiqian Guo*

This journal is © The Royal Society of Chemistry 2025

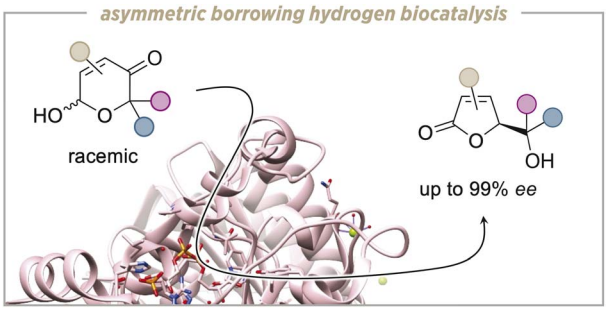
Open Access Article. Published on 01 October 2025. Downloaded on 12/29/2025 8:38:05 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

EDGE ARTICLES

17667

Asymmetric ring contraction of 2-hydroxypyranones by borrowing hydrogen biocatalysis

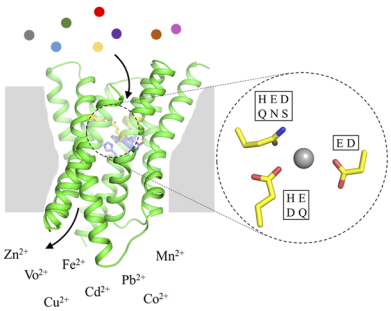
Yuchang Liu,* Adam O'Connell, J. D. Rolfes and Jan Deska*



17675

Targeting the selectivity filter to drastically alter the activity and substrate spectrum of a promiscuous metal transporter

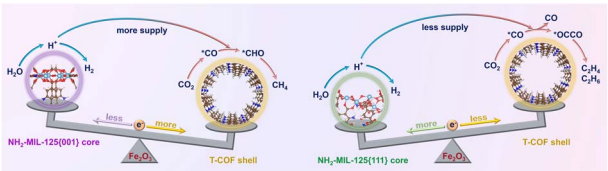
Yuhan Jiang, Michael Nikolovski, Tianqi Wang, Keith MacRenaris, Thomas V. O'Halloran* and Jian Hu*



17688

Facet engineering of MOF supports regulates product selectivity in CO_2 photoreduction by modulating electron and proton supply to COF shells

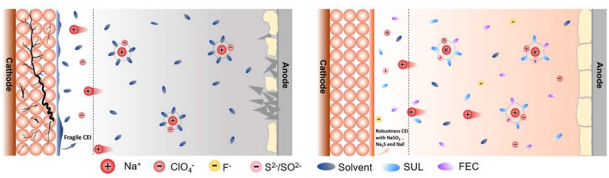
Hulin Shi, Zengrong Li, Shenglan Chen, Yangtao Yao, Linyi Wu, Ruowen Shao, Chang Sheng, Shuxian Zhong, Dongmei Wang, Yuling Zhao, Leihong Zhao and Song Bai*



17703

A bidirectional interfacial engineering strategy for highly stable sodium metal batteries

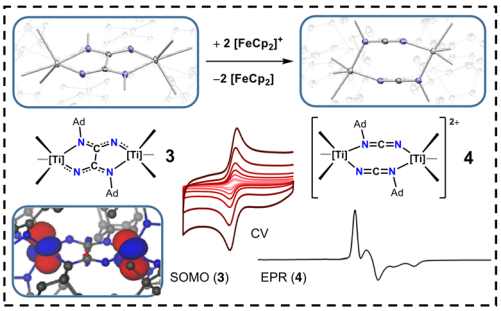
Xiaomin Yang, Long Wang, Minghui Zhao, Lingxiao Peng, Yun Wu, Baohua Zhu,* Le Chen* and Jinliang Li*



Open Access Article. Published on 01 October 2025. Downloaded on 12/29/2025 8:38:05 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

EDGE ARTICLES

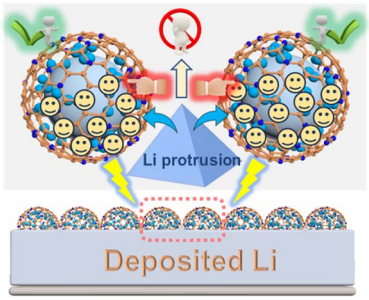
17714



A titanium redox-switch enables reversible C–C bond forming and splitting reactions

Mehrafshan G. Jafari, Dominik Fehn, Christian Sandoval-Pauker, Michael R. Gau, Karsten Meyer,* Balazs Pinter,* Daniel J. Mindiola* and Anders Reinholdt*

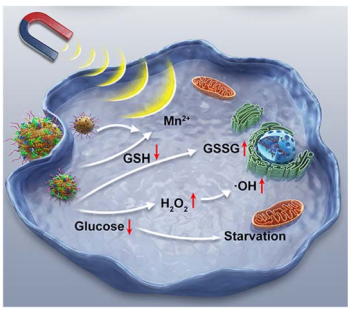
17725



Hierarchical hollow nanospheres of imine-based covalent organic frameworks with built-in Ag sites for fast-charging lithium metal batteries

Tiancun Liu,* Xiao-Meng Lu, Song Lu, Ronghan Jiang, Min Guo, Chaofei Guo,* Zhixin Yu and Yong Wang*

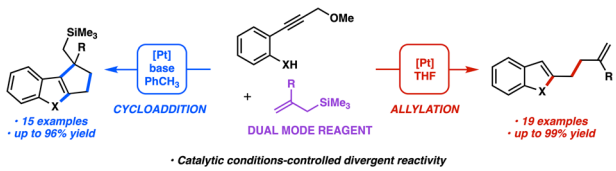
17736



GSH-responsive magnetic imaging for *in situ* monitoring of tumor chemodynamic therapy

Jun Lu, Zhongyao Jiang, Xinyu Chen, Wei Zhang,* Ping Li, Yue Tang,* Wen Zhang, Hui Wang and Bo Tang*

17744



The dichotomous behavior of allylsilanes in the additions to platinum α,β-unsaturated carbenes

Jeff P. Costello, Jacob P. Garber, Khoi Q. Huynh and Eric M. Ferreira*

This journal is © The Royal Society of Chemistry 2025

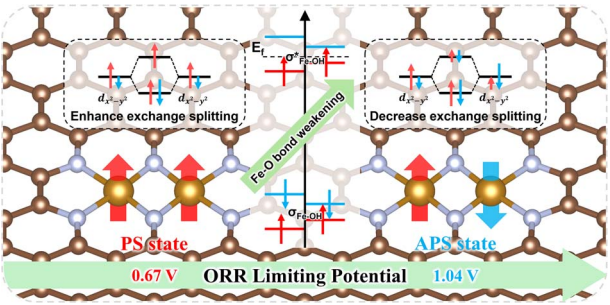
Open Access Article. Published on 01 October 2025. Downloaded on 12/29/2025 8:38:05 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

EDGE ARTICLES

17753

The spin-coupling-dependent oxygen reduction mechanism in dual-atom catalysts

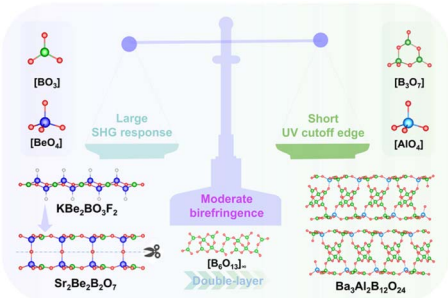
Mingyuan Yu, Erjun Kan* and Cheng Zhan*



17766

$Ba_3Al_2B_{12}O_{24}$: a beryllium-free member of the $Sr_2Be_2B_2O_7$ family with a $^2_\infty[B_{12}Al_2O_{28}]$ double-layered structure

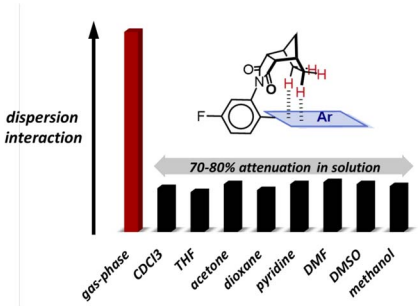
Xiaorong Liu, Hongping Wu,* Zhanggui Hu, Jiyang Wang, Yicheng Wu and Hongwei Yu*



17772

Solvent attenuation of dispersion interactions quantified in polar and nonpolar media using rigid CH–π balances

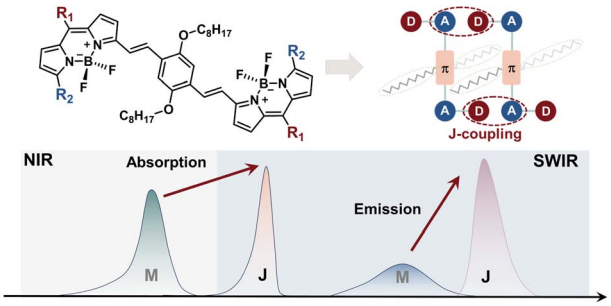
Hao Liu, Harrison M. Scott, Binzhou Lin, Xiaolong Huang, Mark D. Smith and Ken D. Shimizu*



17779

Shortwave infrared absorbing and fluorescent BODIPY J-aggregates for high-contrast *in vivo* imaging

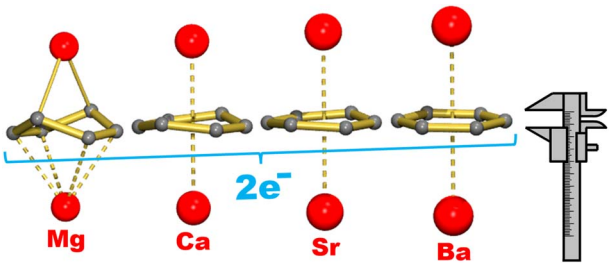
Zhiyong Jiang, Xiangjun Ma, Kaixuan Song, Tianzhu Wang, Mengxi Dong, Hang Liu, Hu Gao, Xiaoqing Wang,* Jing Zhao* and Zhipeng Liu*



Open Access Article. Published on 01 October 2025. Downloaded on 12/29/2025 8:38:05 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

EDGE ARTICLES

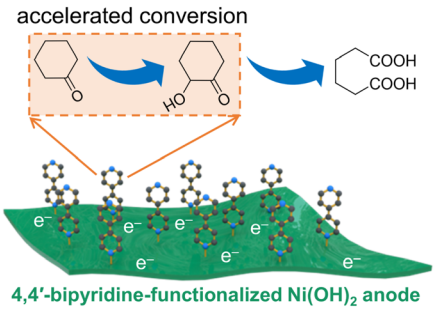
17793



Trends in benzene inverse sandwich complexes of the alkaline-earth metals Mg, Ca, Sr and Ba

Dawid Jędrzkiewicz,* Michael Morasch, Oliver P. E. Townrow, Bastian Rösch, Jens Langer, Zachary Mathe and Sjoerd Harder*

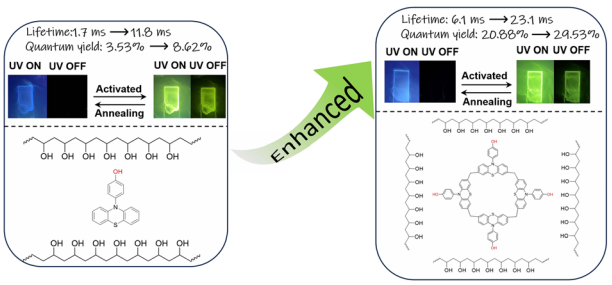
17803



Molecular functionalization of $Ni(OH)_2$ promotes electrosynthesis of adipic acid

Rui Yang, Yuanhao Li, Haonan Xu, Qicheng Zhang, Shufan He, Tao Shen, Xiaobin Fan, Tao Wu* and Yifan Sun*

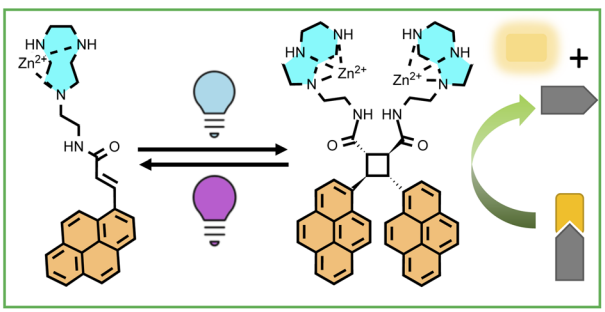
17812



Cyclization-enhanced photoactivatable reversible room-temperature phosphorescence for efficient real-time light printing

Yonghui Sun,* Yuqing Shu, Li Zheng, Yufei Song, Baotong Huang, Xiufang Xu, Haohua Chen,* Junbiao Chang and Pengyang Xin*

17820



Regioselective photodimerization as a tool for light-regulated catalyst assembly

Tommaso Marchetti, Federico Rastrelli, Maohua Lin, Alessandro Negri, Sara Bonacchi, Leonard J. Prins and Luca Gabrielli*

This journal is © The Royal Society of Chemistry 2025

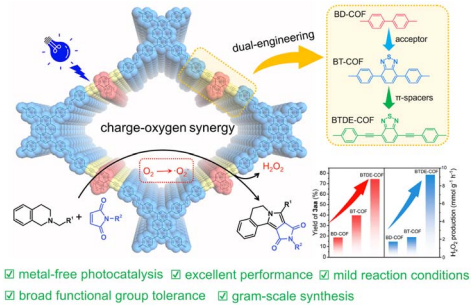
Open Access Article. Published on 01 October 2025. Downloaded on 12/29/2025 8:38:05 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

EDGE ARTICLES

17827

A dual-engineered covalent organic framework with charge-oxygen synergy promotes photocatalytic dipolar [3 + 2] cycloaddition

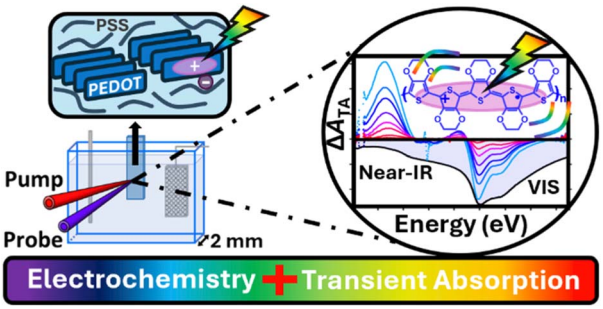
Yuemeng Liu, Lifan Shen, Hao Yang, Xiaojia Zhao and Xingwang Lan*



17839

***In situ* monitoring of polarons in a mixed conducting polymer using ultrafast transient absorption spectroelectrochemistry**

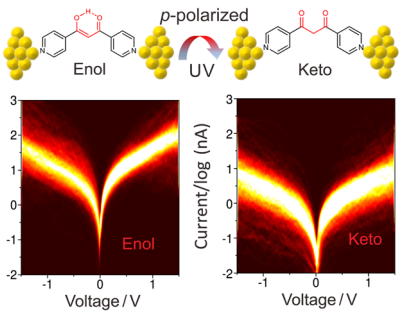
Caitlyn Clark, Abdul Rashid Umar and Christopher Grieco*



17850

Regulating enol–keto tautomerism at the single-molecule level with a confined optical field

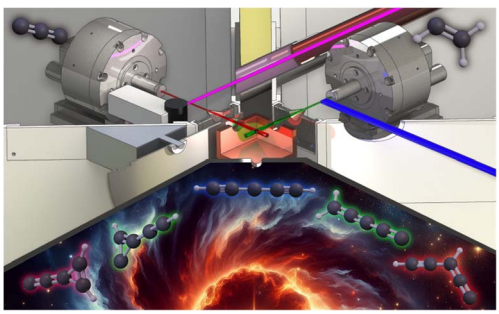
Adila Adijiang, Yunlong Ge, Hefa Feng, Yan Yan, Xin Zuo, Haoyu Wang, Xueyan Zhao, Min Tan, Surong Zhang, Xiaona Xu, Lichuan Chen, Chuankui Wang, Zongliang Li* and Dong Xiang*



17859

From the laboratory to space: unveiling isomeric diversity of C_5H_2 in the reaction of tricarbon (C_3, $X^1\Sigma_g^+$) with the vinyl radical (C_2H_3, X^2A')

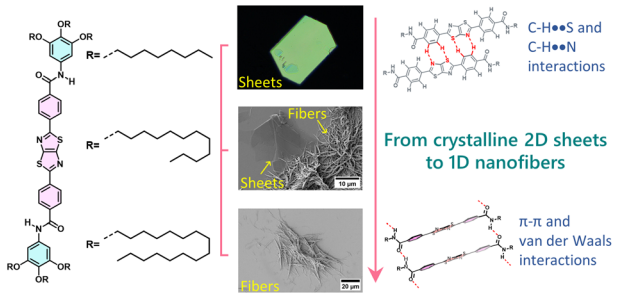
Iakov A. Medvedkov, Anatoliy A. Nikolayev, Shane J. Goettl, Zhenghai Yang, Alexander M. Mebel* and Ralf I. Kaiser*



Open Access Article. Published on 01 October 2025. Downloaded on 12/29/2025 8:38:05 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

EDGE ARTICLES

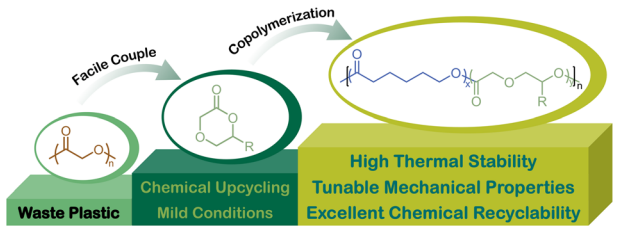
17867



Tuning the dimensionality of functional thiazolo[5,4-*d*]thiazole based supramolecular polymers *via* competitive interactions

Akshay Thorat, Rahul Sahu, Udaijit Pattnaik, Devamrutha Ilayidathu Suresh, Satyaprasad P. Senanayak,* Sandeep K. Reddy* and Chidambar Kulkarni*

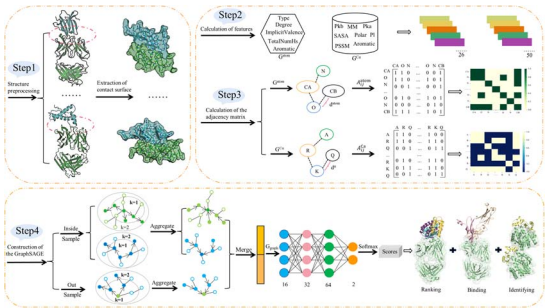
17876



A new paradigm for valorization of waste poly(glycolic acid): facile coupling with epoxides and synthesis of copolyesters with enhanced performance

Feng Ren, Zhuangzhuang Liang, Yifan Jia, Bokun Li, Zhiqiang Sun, Chenyang Hu,* Xuan Pang* and Xuesi Chen

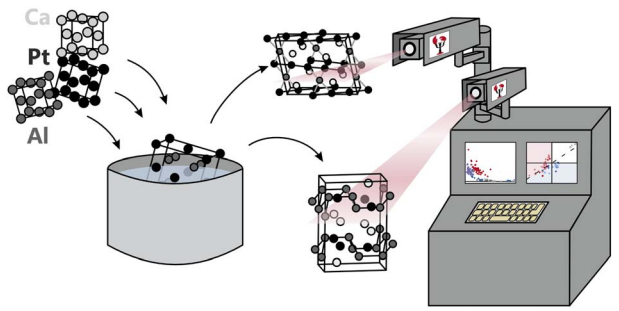
17885



SAGERank: inductive learning of protein–protein interaction from antibody–antigen recognition

Chuance Sun, Xiangyi Li, Honglin Xu, Yike Tang, Ganggang Bai, Yanjing Wang and Buyong Ma*

17900



Differences and similarities in the chemical bonding of intermetallic phases in the Ca–Al–Pt system

Peter C. Müller, Linda S. Reitz, Stefan Engel, Richard Dronskowski* and Oliver Janka*

This journal is © The Royal Society of Chemistry 2025

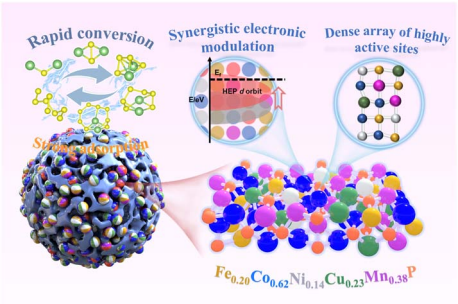
Open Access Article. Published on 01 October 2025. Downloaded on 12/29/2025 8:38:05 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

EDGE ARTICLES

17911

High-entropy metal phosphide nanoparticles for accelerated lithium polysulfide conversion

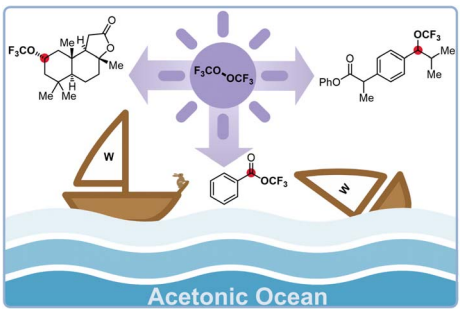
Manchuan Guo, Jin Guo, Tao Ren, Haici Deng, Yanqiu Zhu and Jinliang Zhu*



17921

Photomediated C–H trifluoromethoxylations enabled by bis(trifluoromethyl)peroxide

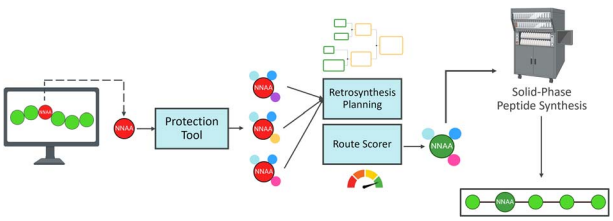
Kamar Shakeri, Merlin Kleoff, Paul Golz, Thomas Drews, Manuela Weber, Sebastian Riedel* and Mathias Christmann*



17927

From concept to chemistry: integrating protection group strategy and reaction feasibility into non-natural amino acid synthesis planning

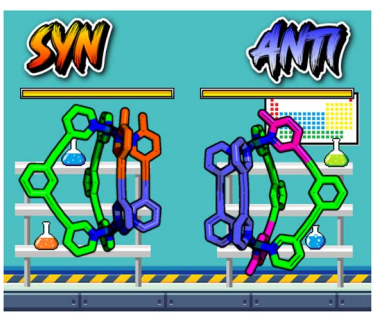
Gökçe Geylan,* Mikhail Kabeshov, Samuel Genheden, Christos Kannas, Thierry Kogej, Leonardo De Maria, Florian David and Ola Engkvist



17939

Coordination sphere interactions drive isomer selection in heteroleptic Pd(II) cages with low-symmetry ligands

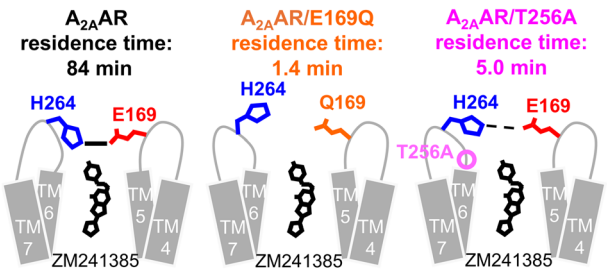
Paulina Molinska, Louise Male and James E. M. Lewis*



Open Access Article. Published on 01 October 2025. Downloaded on 12/29/2025 8:38:05 AM.
This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

EDGE ARTICLES

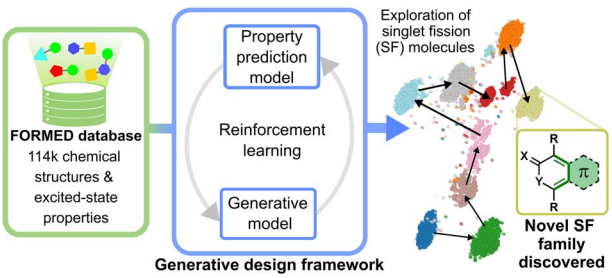
17948



Structural basis of the residence time of adenosine A_{2A} receptor ligands revealed by NMR

Takumi Ueda, Tomoki Tsuchida, Masatoshi Kurita, Takuya Mizumura, Shunsuke Imai, Yutaro Shiraishi, Yutaka Kofuku, Shuhei Miyakawa, Kaori Fukuzawa, Koh Takeuchi and Ichio Shimada*

17956



Generative design of singlet fission materials leveraging a fragment-oriented database

Thanapat Worakul, Rubén Laplaza, J. Terence Blaskovits and Clémence Corminboeuf*

CORRECTION

17970

Correction: Revealing the photocatalytic dissociation of water molecules on rutile TiO_2 surface *via* hybrid functional based linear response time-dependent density functional theory

Lei Wang, Xiaofeng Liu,* Qunxiang Li,* Jinlong Yang and Wei Hu*

This journal is © The Royal Society of Chemistry 2025