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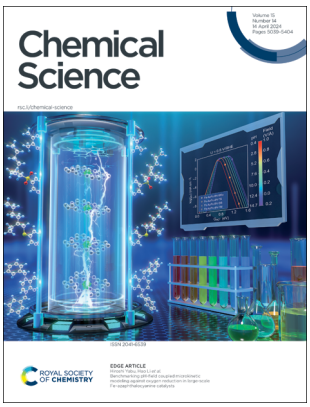
IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(14) 5039–5404 (2024)

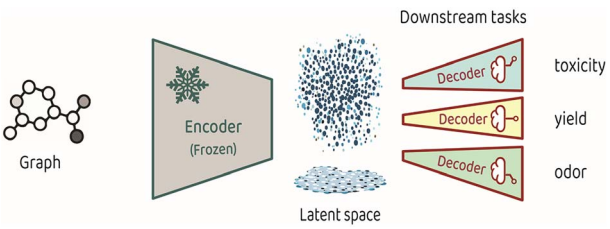
Cover
See Norio Shibata *et al.*, pp. 5113–5122. Image reproduced by permission of Mami Shibata from *Chem. Sci.*, 2024, **15**, 5113. Created by Japanese artist Mami Shibata, titled "Airplane, Treasure-box & Engi-kumade" (bring good luck and prosperity).



Inside cover
See Hiroshi Yabu, Hao Li *et al.*, pp. 5123–5132. Image reproduced by permission of Hao Li from *Chem. Sci.*, 2024, **15**, 5123.

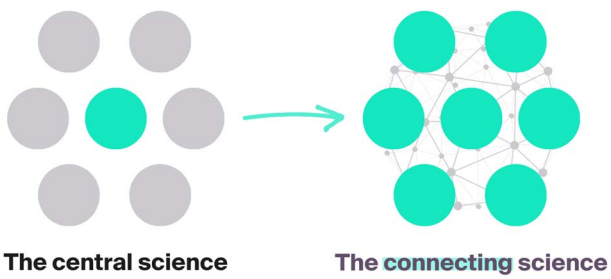
COMMENTARY

5052
A focus on molecular representation learning for the prediction of chemical properties
Yonatan Harnik and Anat Milo*



PERSPECTIVE

5056
Connecting chemical worlds for a sustainable future
Fernando Gomollón-Bel and Javier García-Martínez*



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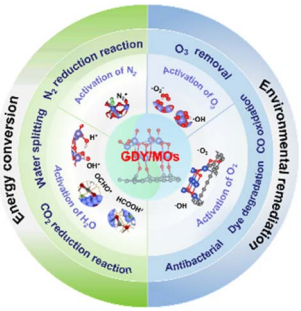
REVIEWS

5061

Graphdiyne/metal oxide hybrid materials for efficient energy and environmental catalysis

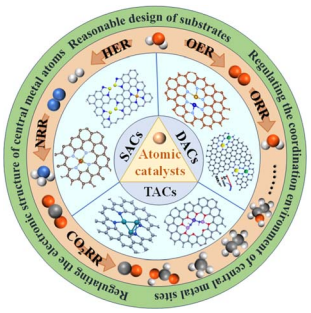
Yuhua Zhu, Shuhong Zhang, Xiaofeng Qiu, Quanguo Hao, Yan Wu, Zhu Luo* and Yanbing Guo*



5082

Structural engineering of atomic catalysts for electrocatalysis

Tianmi Tang, Xue Bai, Zhenlu Wang and Jingqi Guan*

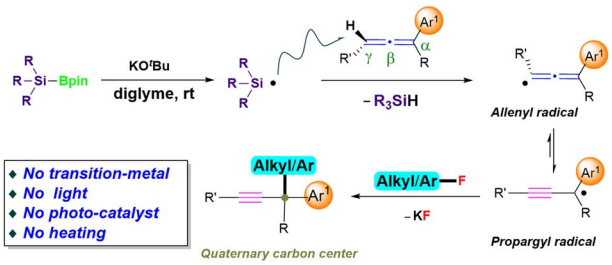


EDGE ARTICLES

5113

Cross-coupling of organic fluorides with allenes: a silyl-radical-relay pathway for the construction of α-alkynyl-substituted all-carbon quaternary centres

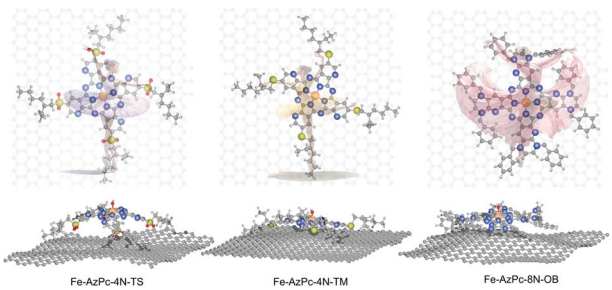
Jun Zhou, Zhengyu Zhao, Soichiro Mori, Katsuhiro Yamamoto and Norio Shibata*



5123

Benchmarking pH-field coupled microkinetic modeling against oxygen reduction in large-scale Fe–azaphthalocyanine catalysts

Di Zhang, Yutaro Hirai, Koki Nakamura, Koju Ito, Yasutaka Matsuo, Kosuke Ishibashi, Yusuke Hashimoto, Hiroshi Yabu* and Hao Li*



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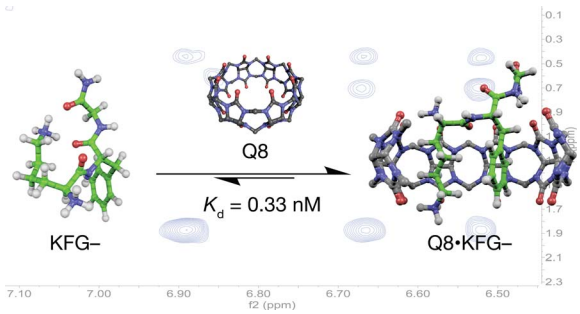
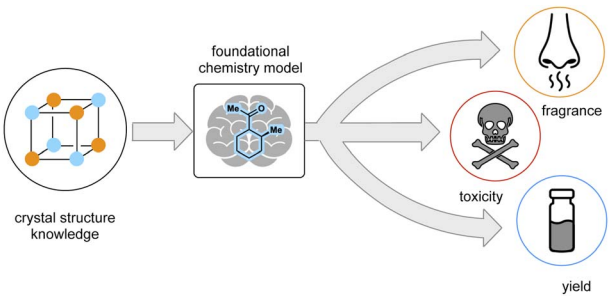


Peptide recognition by a synthetic receptor at subnanomolar concentrations

Paolo Suating, Marc B. Ewe, Lauren B. Kimberly, Hadi D. Arman, Daniel J. Wherritt and Adam R. Urbach*

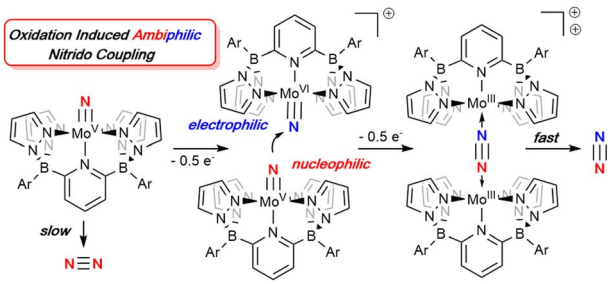
5143



Transfer learning for a foundational chemistry model

Emma King-Smith*

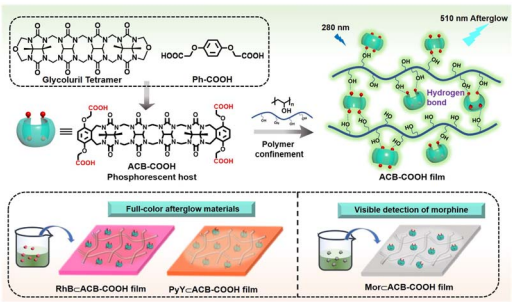
5152



Oxidation-induced ambiphilicity triggers N–N bond formation and dinitrogen release in octahedral terminal molybdenum(v) nitrido complexes

C. Christopher Almquist, Thayalan Rajeshkumar, H. D. A. Chathumal Jayaweera, Nicole Removski, Wen Zhou, Benjamin S. Gelfand, Laurent Maron* and Warren E. Piers*

5163



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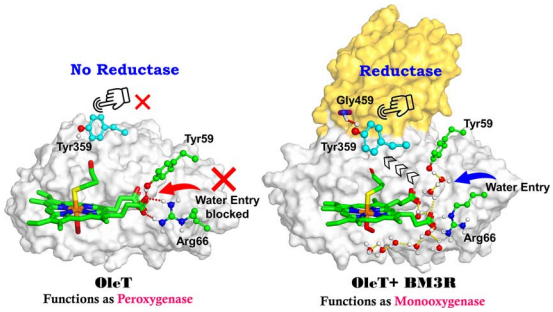
5174

On the engineering of reductase-based-monooxygenase activity in CYP450 peroxygenases

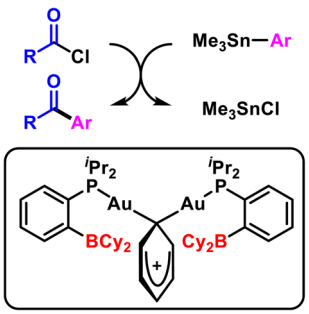
Shalini Yadav, Sason Shaik* and Kshatresh Dutta Dubey*



5187

Chemo-selective Stille-type coupling of acyl-chlorides upon phosphine-borane Au(I) catalysis

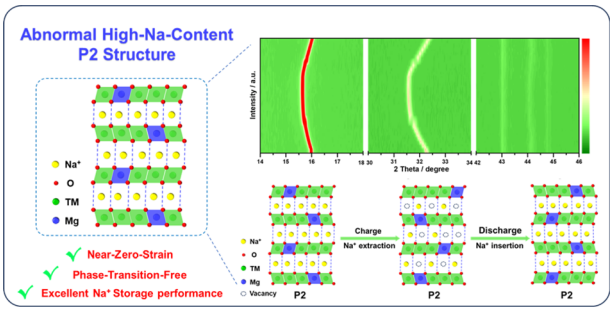
Nereida Hidalgo, Arnaud Le Gac, Sonia Mallet-Ladeira, Ghenwa Bouhadir* and Didier Bourissou*



5192

Developing an abnormal high-Na-content P2-type layered oxide cathode with near-zero-strain for high-performance sodium-ion batteries

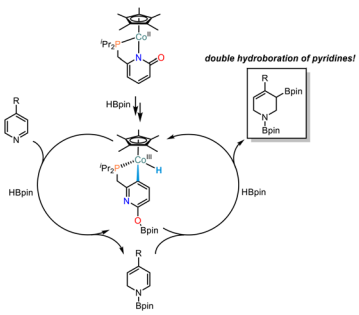
Hai-Yan Hu, Jia-Yang Li, Yi-Feng Liu, Yan-Fang Zhu,* Hong-Wei Li, Xin-Bei Jia, Zhuang-Chun Jian, Han-Xiao Liu, Ling-Yi Kong, Zhi-Qi Li, Hang-Hang Dong, Meng-Ke Zhang, Lang Qiu, Jing-Qiang Wang, Shuang-Qiang Chen, Xiong-Wei Wu, Xiao-Dong Guo and Yao Xiao*



5201

Cobalt-catalyzed double hydroboration of pyridines

Finn Höeg, Lea Luxenberger, Andrey Fedulin* and Axel Jacobi von Wangelin*



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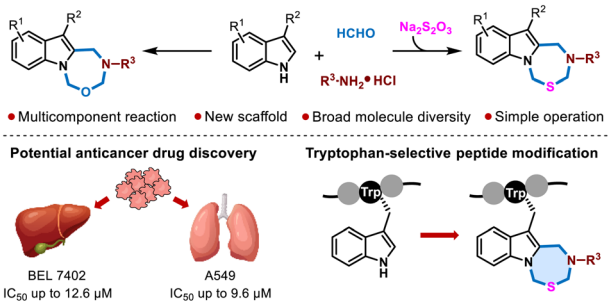
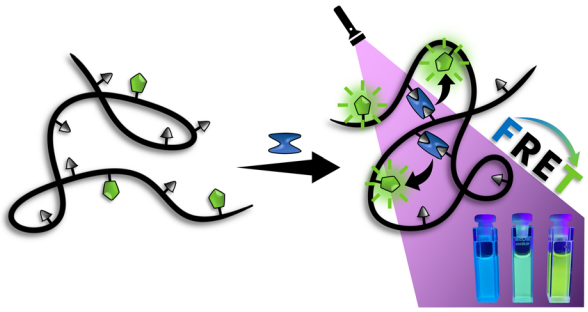


A multicomponent reaction for modular assembly of indole-fused heterocycles

Jiaming Li, Hao Ni, Weiwei Zhang, Zhencheng Lai, Huimin Jin, Linwei Zeng* and Sunliang Cui*

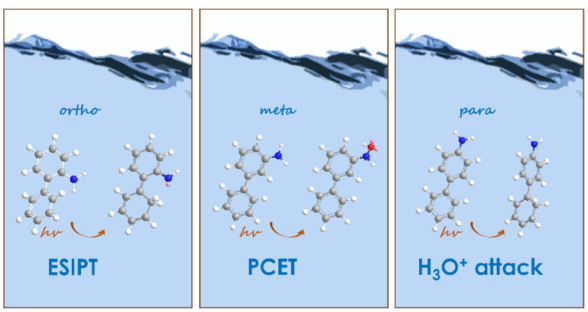
5218



Förster resonance energy transfer within single chain nanoparticles

Patrick H. Maag, Florian Feist, Hendrik Frisch,* Peter W. Roesky* and Christopher Barner-Kowollik*

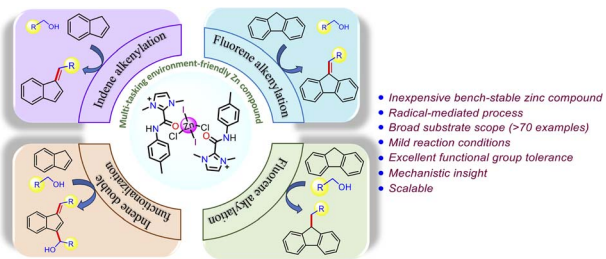
5225



Excited-state antiaromaticity relief drives facile photoprotonation of carbons in aminobiphenyls

Josip Draženović, Croix J. Laconsay, Nađa Došlić,* Judy I-Chia Wu* and Nikola Basarić*

5238



Unravelling a bench-stable zinc-amide compound as highly active multitasking catalyst for radical-mediated selective alk(en)ylation of unactivated carbocycles under mild conditions

Sangita Sahoo, Subarna Manna and Arnab Rit*

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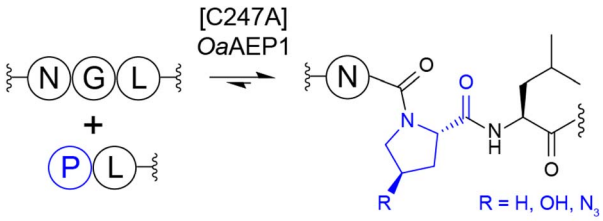
5248

Tertiary amide bond formation by an engineered asparaginyl ligase

Simon J. de Veer,* Yan Zhou, Thomas Durek, David J. Craik* and Fabian B. H. Rehm*

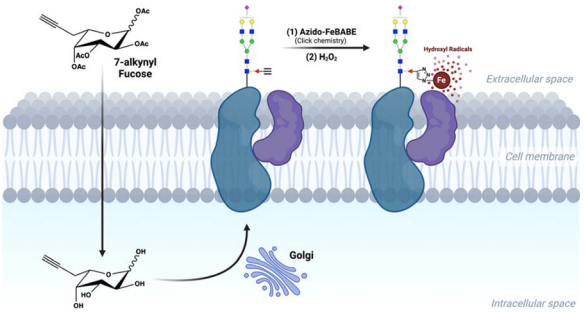


✓ Ligase-catalysed tertiary amide bond synthesis
✓ One-pot dual labelling directly at the ligation junction

5256

Protein oxidation of fucose environments (POFE) reveals fucose–protein interactions

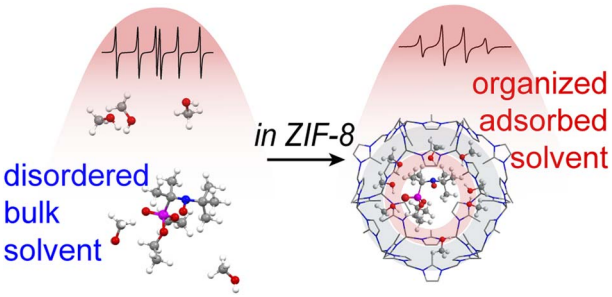
Yixuan Xie, Siyu Chen, Michael Russelle Alvarez, Ying Sheng, Qiongyu Li, Emanual Maverakis and Carlito B. Lebrilla*



5268

Nanoscale solvent organization in metal–organic framework ZIF-8 probed by EPR of flexible β-phosphorylated nitroxides

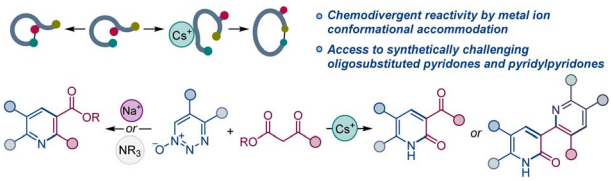
Artem S. Poryvaev, Aleksandr A. Efremov, Dmitry V. Alimov, Kristina A. Smirnova, Daniil M. Polyukhov, Renad Z. Sagdeev, Samuel Jacoutot, Sylvain R. A. Marque* and Matvey V. Fedin*



5277

The "cesium effect" magnified: exceptional chemoselectivity in cesium ion mediated nucleophilic reactions

Soumen Biswas, William B. Hughes, Luca De Angelis, Graham C. Haug, Ramon Trevino, Seth O. Fremin, Hadi D. Arman, Oleg V. Larionov* and Michael P. Doyle*



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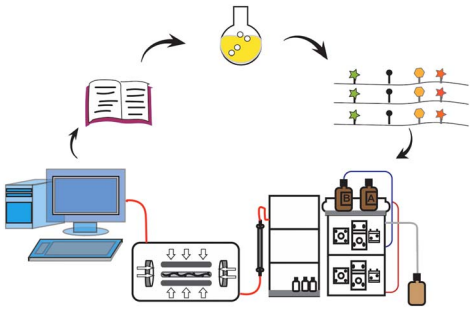
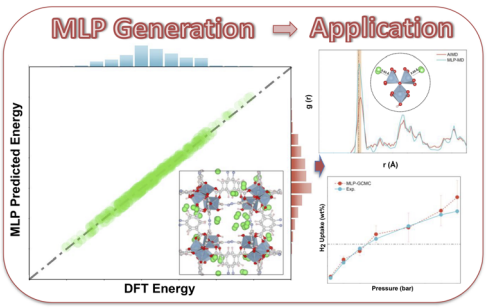


Chemical and linguistic considerations for encoding Chinese characters: an embodiment using chain-end degradable sequence-defined oligourethanes created by consecutive solid phase click chemistry

Le Zhang, Todd B. Krause, Harnimarta Deol, Bipin Pandey, Qifan Xiao, Hyun Meen Park, Brent L. Iverson,* Danny Law* and Eric V. Anslyn*

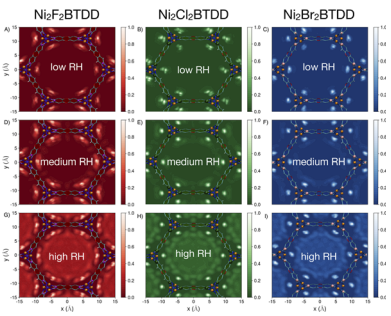
5294



Machine learning potential for modelling H_2 adsorption/diffusion in MOFs with open metal sites

Shanping Liu, Romain Dupuis, Dong Fan, Salma Benzaria, Mickaele Bonneau, Prashant Bhatt, Mohamed Eddaoudi* and Guillaume Maurin*

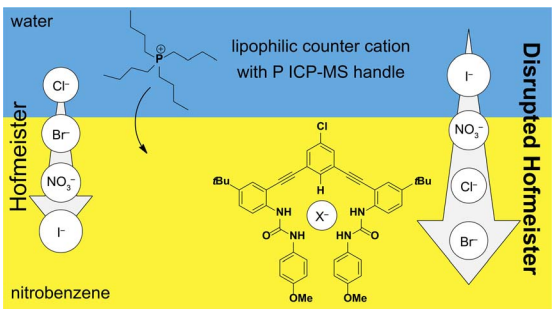
5303



Monitoring water harvesting in metal–organic frameworks, one water molecule at a time

Kelly M. Hunter and Francesco Paesani*

5311



Disrupting the Hofmeister bias in salt liquid–liquid extraction with an arylethynyl bisurea anion receptor

Hazel A. Fargher, Lætitia H. Delmau, Vyacheslav S. Bryantsev, Michael M. Haley,* Darren W. Johnson* and Bruce A. Moyer*

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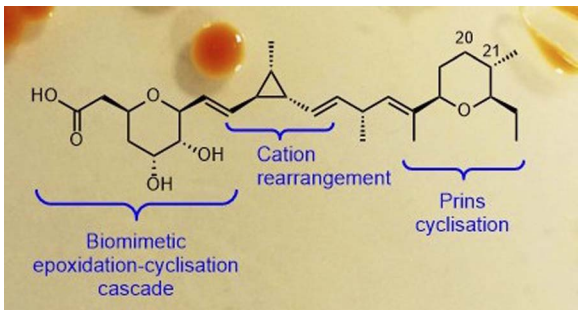
5319

Combining total synthesis and genetic engineering to probe dihydropyran formation in ambruticin biosynthesis

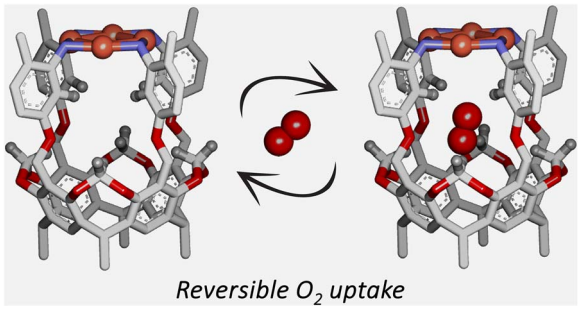
James I. Bowen, Xiaotong Zhong, Kaining Gao, Benjamin Reed, Matthew P. Crump, Luoyi Wang* and Christine L. Willis*



5327

Reversible dioxygen uptake at [Cu_4] clusters

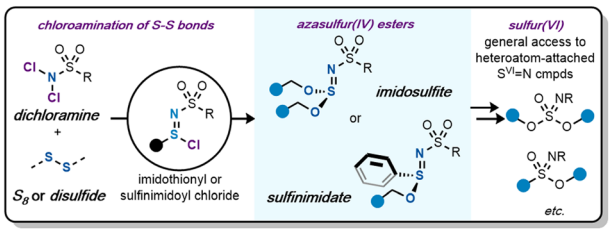
Manasseh Kusi Osei, Saber Mirzaei, M. Saeed Mirzaei, Agustin Valles and Raúl Hernández Sánchez*



5333

Azasulfur(IV) derivatives of sulfite and sulfinate esters by formal S–S bond insertion of dichloramines

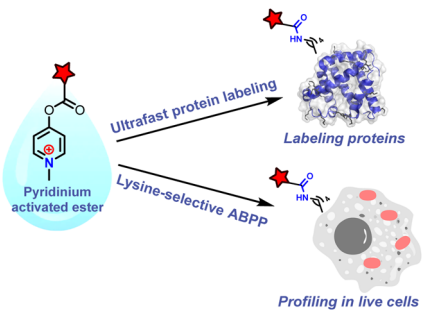
Peng Wu, Joachim Demaerel, Benjamin J. Statham and Carsten Bolm*



5340

A pyridinium-based strategy for lysine-selective protein modification and chemoproteomic profiling in live cells

Chuan Wan, Dongyan Yang, Chunli Song, Mingchan Liang, Yuhao An, Chenshan Lian, Chuan Dai, Yuxin Ye, Feng Yin,* Rui Wang* and Zigang Li*



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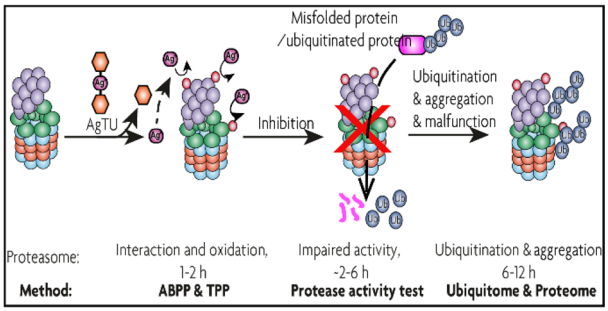
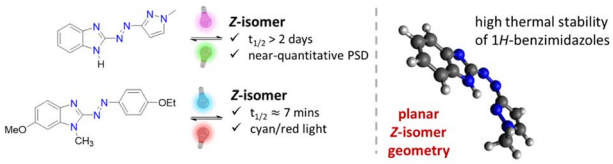


Integrative chemoproteomics reveals anticancer mechanisms of silver(I) targeting the proteasome regulatory complex

Xiaojian Shao, Fangrong Xing, Yiwei Zhang, Chun-Nam Lok and Chi-Ming Che*

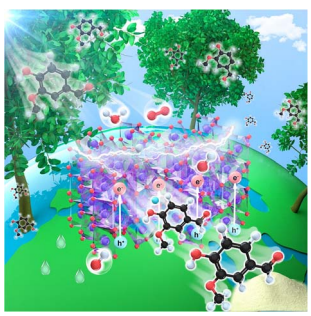
5360



Arylazobenzimidazoles: versatile visible-light photoswitches with tuneable *Z*-isomer stability

Sophie A. M. Steinmüller, Magdalena Odaybat, Giulia Galli, Davia Prischich, Matthew J. Fuchter* and Michael Decker*

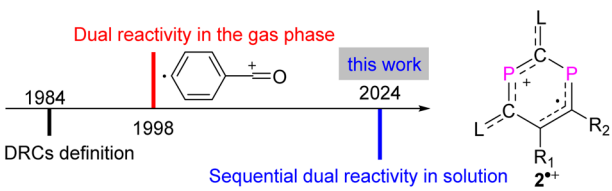
5368



Sunlight-driven and gram-scale vanillin production *via* Mn-defected γ-MnO_2 catalyst in aqueous environment

Qingping Ke, Yurong Zhang, Chao Wan,* Jun Tang, Shenglai Li, Xu Guo, Minsu Han,* Takashi Hamada, Sameh M. Osman, Yunqing Kang* and Yusuke Yamauchi

5376



Sequential radical and cationic reactivity at separated sites within one molecule in solution

Shihua Liu, Yinwu Li, Jieli Lin, Zhuofeng Ke, Hansjörg Grützmacher, Cheng-Yong Su and Zhongshu Li*

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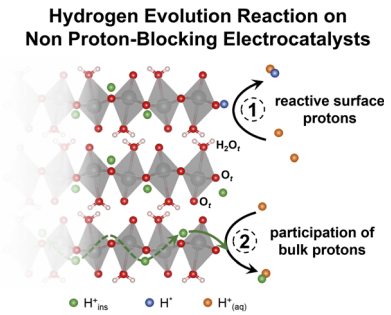
5385

Participation of electrochemically inserted protons in the hydrogen evolution reaction on tungsten oxides

Michael A. Spencer, Noah P. Holzapfel, Kyung-Eun You, Giannis Mpourmpakis and Veronica Augustyn*



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