

Chemical Science

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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

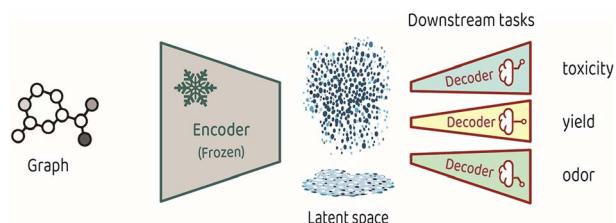
See Hiroshi Yabu, Hao Li et al., pp. 5123–5132. Image reproduced by permission of Hao Li from *Chem. Sci.*, 2024, 15, 5123.

COMMENTARY

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A focus on molecular representation learning for the prediction of chemical properties

Yonatan Harnik and Anat Milo*

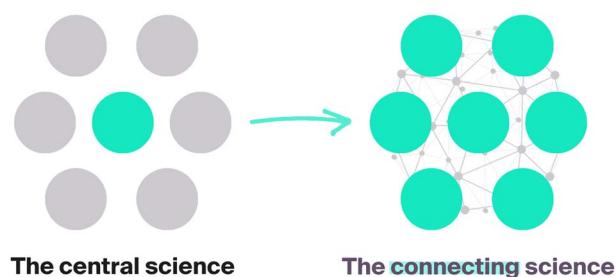


PERSPECTIVE

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Connecting chemical worlds for a sustainable future

Fernando Gomollón-Bel and Javier García-Martínez*



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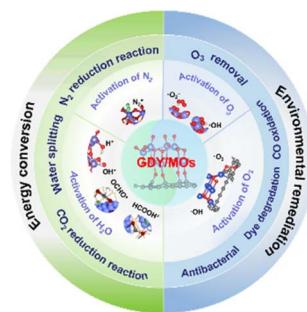
Fundamental questions
Elemental answers

REVIEWS

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

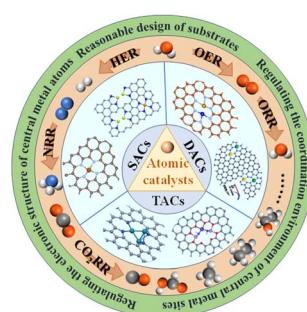
Yuhua Zhu, Shuhong Zhang, Xiaofeng Qiu, Quanguo Hao, Yan Wu, Zhu Luo* and Yanbing Guo*



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Structural engineering of atomic catalysts for electrocatalysis

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

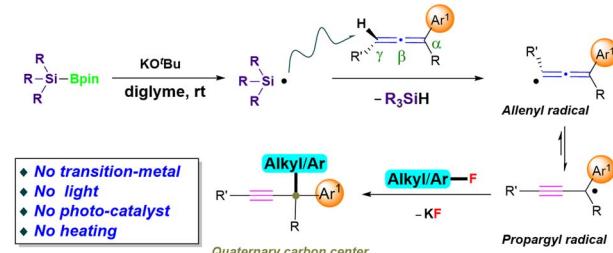


EDGE ARTICLES

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

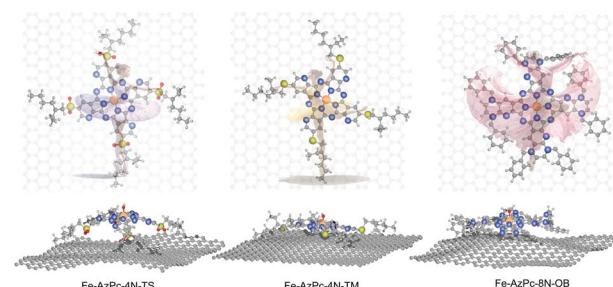
Jun Zhou, Zhengyu Zhao, Soichiro Mori, Katsuhiro Yamamoto and Norio Shibata*



5123

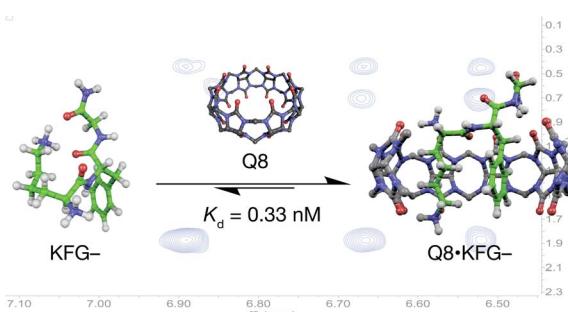
Benchmarking pH-field coupled microkinetic modeling against oxygen reduction in large-scale Fe–azaphthalocyanine catalysts

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



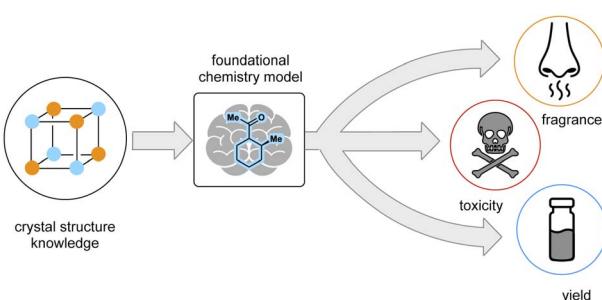
EDGE ARTICLES

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**Peptide recognition by a synthetic receptor at subnanomolar concentrations**

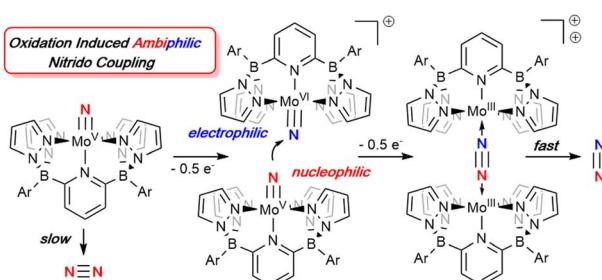
Paolo Suating, Marc B. Ewe, Lauren B. Kimberly, Hadi D. Arman, Daniel J. Wherritt and Adam R. Urbach*

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**Transfer learning for a foundational chemistry model**

Emma King-Smith*

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**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*

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**Phosphorescent acyclic cucurbituril solid supramolecular multicolour delayed fluorescence behaviour**

Man Huo, Shuang-Qi Song, Xian-Yin Dai, Fan-Fan Li, Yu-Yang Hu and Yu Liu*

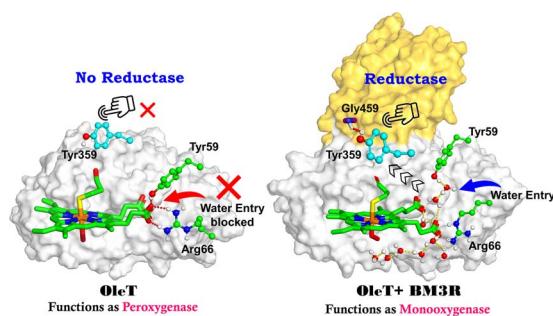


EDGE ARTICLES

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

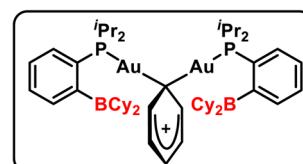
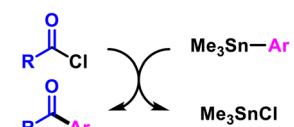
Shalini Yadav, Sason Shaik* and Kshatresh Dutta Dubey*



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

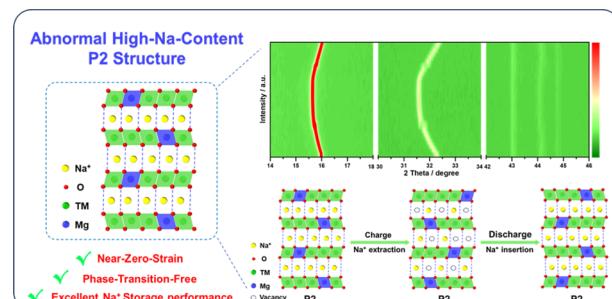
Nereida Hidalgo, Arnaud Le Gac, Sonia Mallet-Ladeira, Ghenwa Bouhadir* and Didier Bourissou*



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

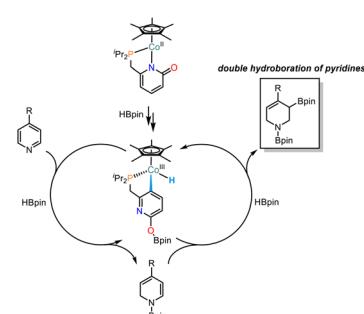
Hai-Yan Hu, Jia-Yang Li, Yi-Feng Liu, Yan-Fang Zhu,* Hong-Wei Li, Xin-Bei Jia, Zhuang-Chun Jian, Han-Xiao Liu, Ling-Yi Kong, Zhi-Qi Li, Hang-Hang Dong, Meng-Ke Zhang, Lang Qiu, Jing-Qiang Wang, Shuang-Qiang Chen, Xiong-Wei Wu, Xiao-Dong Guo and Yao Xiao*



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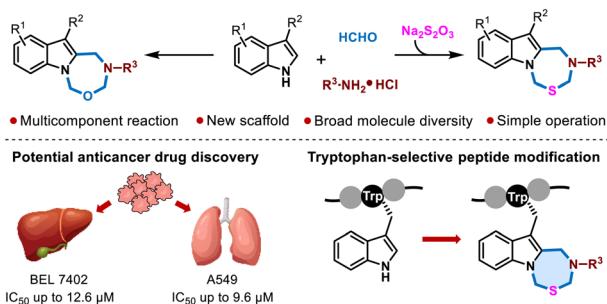
Cobalt-catalyzed double hydroboration of pyridines

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



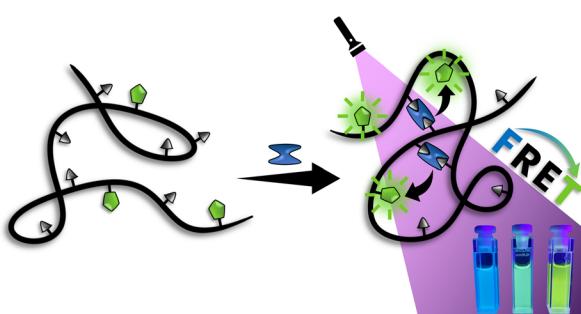
EDGE ARTICLES

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**A multicomponent reaction for modular assembly of indole-fused heterocycles**

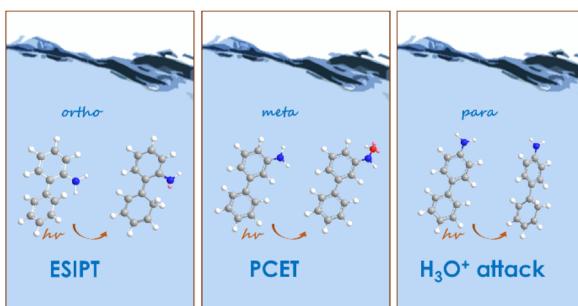
Jiaming Li, Hao Ni, Weiwei Zhang, Zhencheng Lai, Huimin Jin, Linwei Zeng* and Sunliang Cui*

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**Förster resonance energy transfer within single chain nanoparticles**

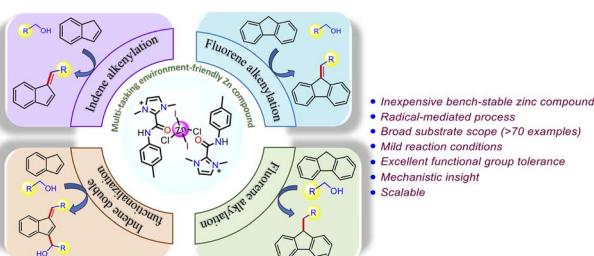
Patrick H. Maag, Florian Feist, Hendrik Frisch,* Peter W. Roesky* and Christopher Barner-Kowollik*

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

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

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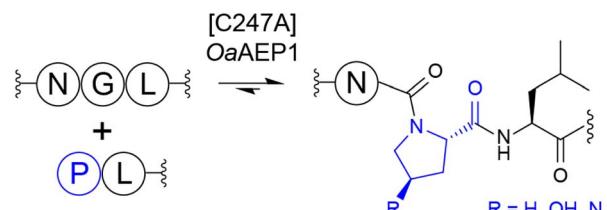
**Unravelling a bench-stable zinc-amide compound as highly active multitasking catalyst for radical-mediated selective alk(en)ylation of unactivated carbocycles under mild conditions**

Sangita Sahoo, Subarna Manna and Arnab Rit*



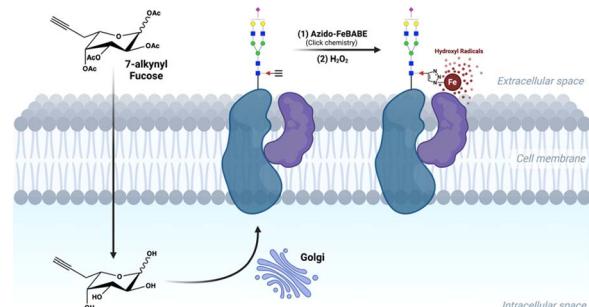
EDGE ARTICLES

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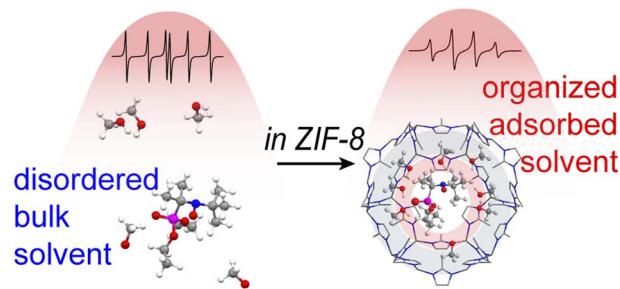
Tertiary amide bond formation by an engineered asparaginyl ligaseSimon J. de Veer,* Yan Zhou, Thomas Durek,
David J. Craik* and Fabian B. H. Rehm*

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

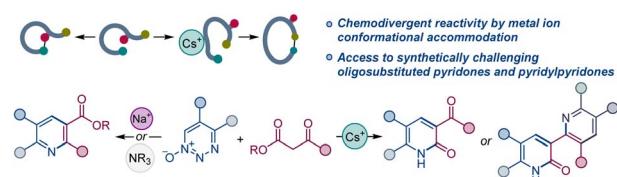
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Protein oxidation of fucose environments (POFE) reveals fucose–protein interactionsYixuan Xie, Siyu Chen, Michael Russelle Alvarez,
Ying Sheng, Qiongyu Li, Emanuel Maverakis and
Carlito B. Lebrilla*

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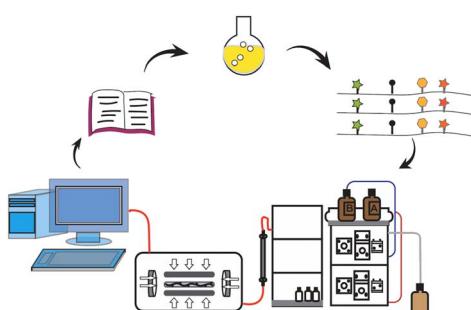
Nanoscale solvent organization in metal–organic framework ZIF-8 probed by EPR of flexible β -phosphorylated nitroxidesArtem S. Poryvaev, Aleksandr A. Efremov,
Dmitry V. Alimov, Kristina A. Smirnova,
Daniil M. Polyukhov, Renad Z. Sagdeev, Samuel Jacoutot,
Sylvain R. A. Marque* and Matvey V. Fedin*

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The “cesium effect” magnified: exceptional chemoselectivity in cesium ion mediated nucleophilic reactionsSoumen 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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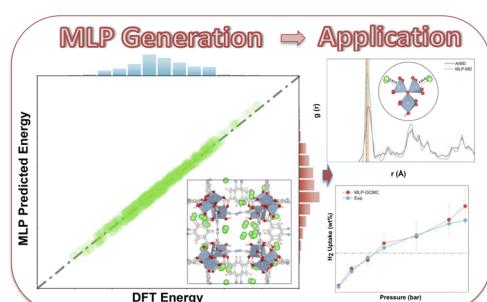
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Chemical and linguistic considerations for encoding Chinese characters: an embodiment using chain-end degradable sequence-defined oligourethanes created by consecutive solid phase click chemistry

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

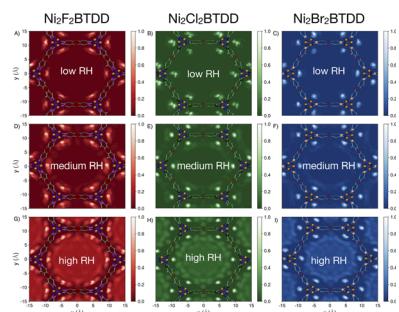
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Machine learning potential for modelling H₂ adsorption/diffusion in MOFs with open metal sites

Shaping Liu, Romain Dupuis, Dong Fan, Salma Benzaria, Mickaële Bonneau, Prashant Bhatt, Mohamed Eddaoudi^{*} and Guillaume Maurin^{*}

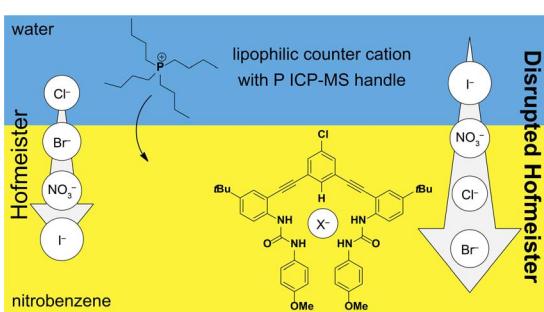
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Monitoring water harvesting in metal–organic frameworks, one water molecule at a time

Kelly M. Hunter and Francesco Paesani^{*}

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

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

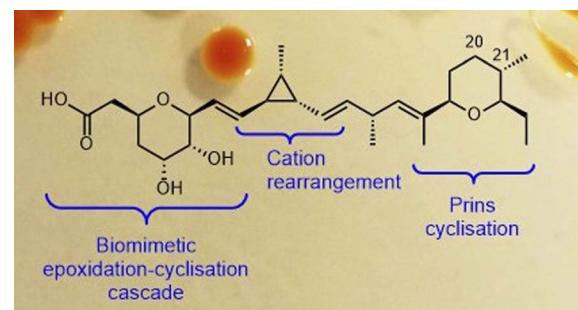


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Combining total synthesis and genetic engineering to probe dihydropyran formation in ambruticin biosynthesis

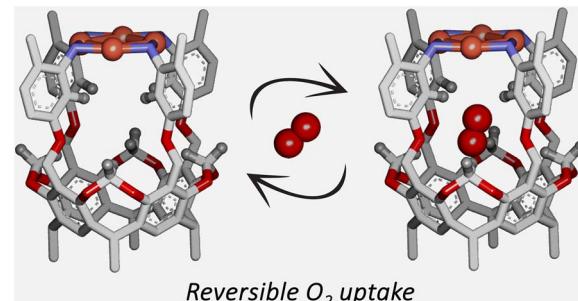
James I. Bowen, Xiaotong Zhong, Kaining Gao,
Benjamin Reed, Matthew P. Crump, Luoyi Wang*
and Christine L. Willis*



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Reversible dioxygen uptake at $[Cu_4]$ clusters

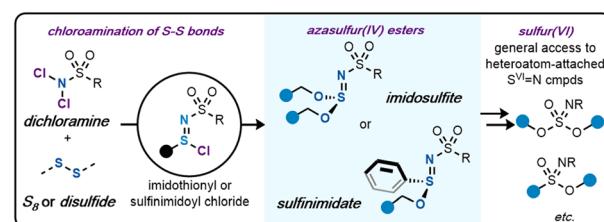
Manasseh Kusi Osei, Saber Mirzaei, M. Saeed Mirzaei,
Agustín Valles and Raúl Hernández Sánchez*



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

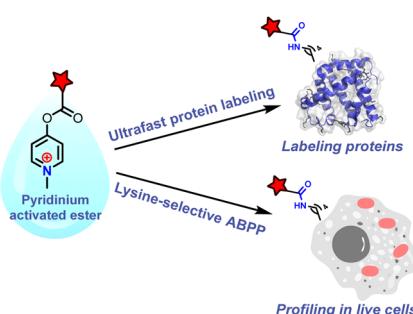
Peng Wu, Joachim Demaerel, Benjamin J. Statham
and Carsten Bolm*



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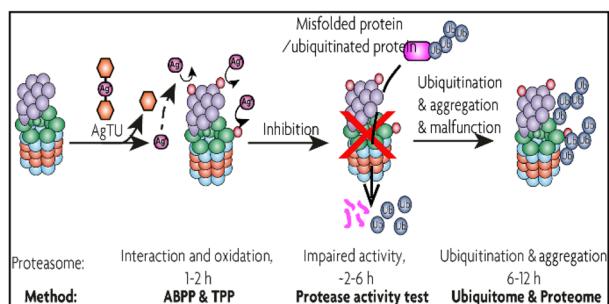
A pyridinium-based strategy for lysine-selective protein modification and chemoproteomic profiling in live cells

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



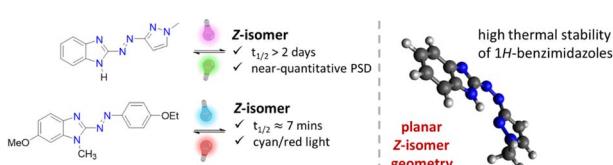
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**Integrative chemoproteomics reveals anticancer mechanisms of silver(i) targeting the proteasome regulatory complex**

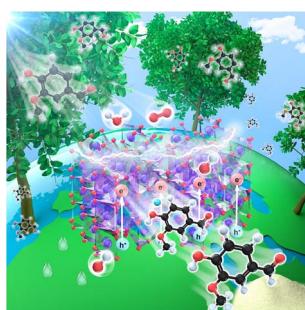
Xiaojian Shao, Fangrong Xing, Yiwei Zhang, Chun-Nam Lok and Chi-Ming Che*

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

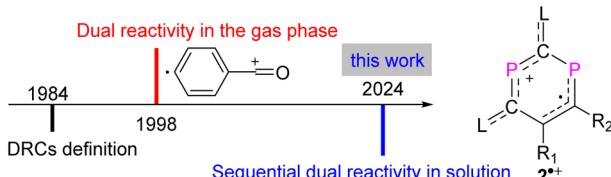
Sophie A. M. Steinmüller, Magdalena Odaybat, Giulia Galli, Davia Prischich, Matthew J. Fuchter* and Michael Decker*

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**Sunlight-driven and gram-scale vanillin production via Mn-defected γ -MnO₂ 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

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

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



EDGE ARTICLES

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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*

Hydrogen Evolution Reaction on Non Proton-Blocking Electrocatalysts