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IN THIS ISSUE

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Cover
See Dirk De Vos *et al.*, pp. 2573–2580. Image reproduced by permission of Joris Snaet from *Chem. Sci.*, 2025, **16**, 2573.

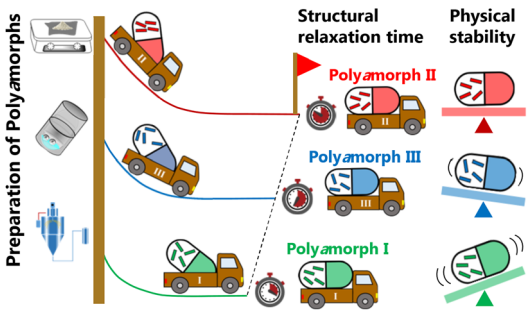
Inside cover
See Rubicelia Vargas, Jorge Garza, Nak Cheon Jeong *et al.*, pp. 2581–2588. Image reproduced by permission of Nak Cheon Jeong from *Chem. Sci.*, 2025, **16**, 2581.

COMMENTARY

2480

A focus on chasing pharmaceutical polyamorphs to design better oral drug formulations

Ana M. Belenguer

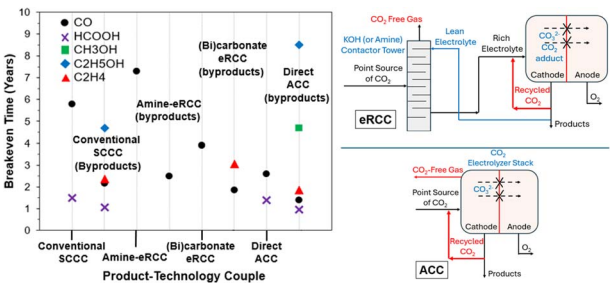


PERSPECTIVE

2483

A critical appraisal of advances in integrated CO_2 capture and electrochemical conversion

Ahmed Badreldin and Ying Li*



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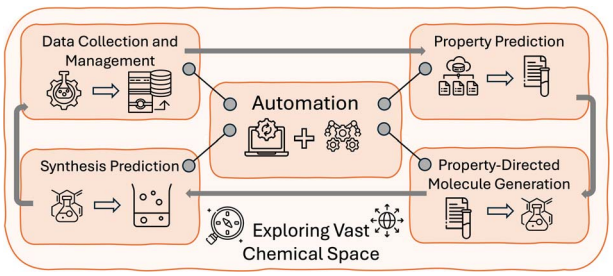
REVIEW

2514

A review of large language models and autonomous agents in chemistry

Mayk Caldas Ramos, Christopher J. Collison and Andrew D. White*

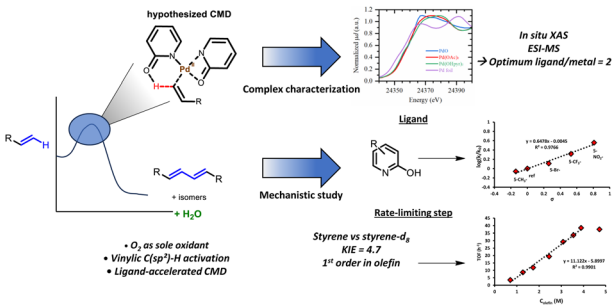


EDGE ARTICLES

2573

Palladium-catalyzed aerobic homocoupling of aliphatic olefins to dienes: evidence for rate-limiting concerted metalation–deprotonation

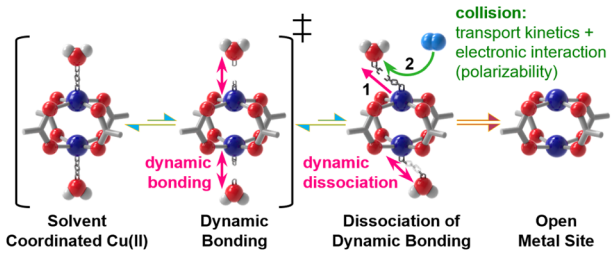
Sam Van Minnebruggen, Harry Poels-Ryckeboer, Hendrik Van Dessel, Frederick Martens, Wouter Stuyck, Tom Nelis, Igor Beckers, Aram Bugaev and Dirk De Vos*



2581

Gas-flow activation of MOFs: unlocking efficient catalysis through dynamic bonding

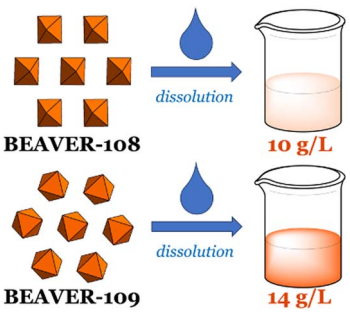
Mariana L. Díaz-Ramírez, Sun Ho Park, Marcos Rivera-Almazo, Erika Medel, Ricardo A. Peralta, Ilich A. Ibarra, Rubicelia Vargas,* Jorge Garza* and Nak Cheon Jeong*



2589

Solvatomorphic diversity dictates the stability and solubility of metal–organic polyhedra

Ankit K. Yadav, Andrzej Gładysiak,* Emma H. Wolpert, Alex M. Ganose, Bronson Samel-Garloff, Dipankar Koley, Kim E. Jelfs and Kyriakos C. Stylianou*



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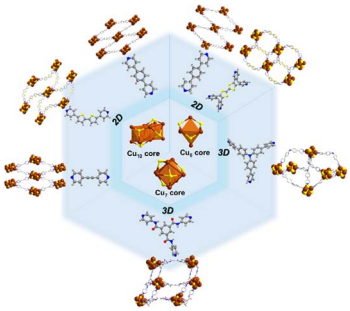
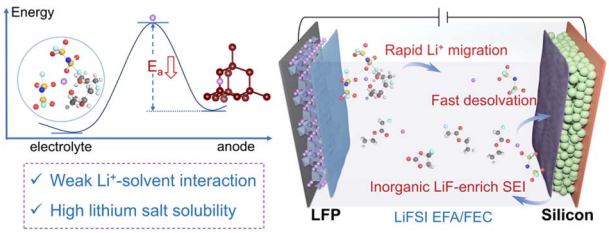


Tunable structural rearrangement in Cu cluster assemblies through linker and solvent alterations

Saikat Das, Jin Sakai, Riki Nakatani, Ayumu Kondo, Rina Tomioka, Subhabrata Das, Shuntaro Takahashi, Tokuhisa Kawawaki, Sourav Biswas* and Yuichi Negishi*

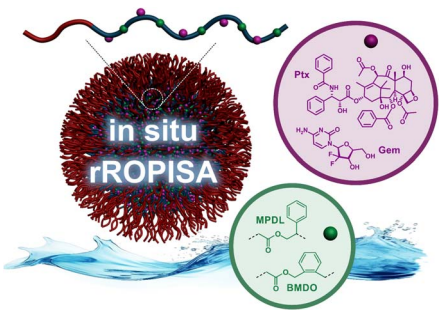
2609



Electrolyte design weakens lithium-ion solvation for a fast-charging and long-cycling Si anode

Min Li, Shuai Li, Dong Yan, Yuhao Ma, Xiaobin Niu and Liping Wang*

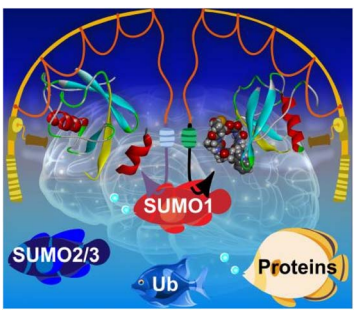
2619



***In situ* synthesis of degradable polymer prodrug nanoparticles**

Chen Zhu, Hannah Beauseroy, Julie Mougin, Maëlle Lages and Julien Nicolas*

2634



Deciphering the endogenous SUMO-1 landscape: a novel combinatorial peptide enrichment strategy for global profiling and disease association

Xiaoyu Zhang, Bowen Zhong, Yue Sun, Dan Liu, Xiancheng Zhang, Dongdong Wang, Cunli Wang, Huiling Gao, Manli Zhong, Haijuan Qin, Yang Chen, Zhiying Yang, Yan Li, Haijie Wei, Xindi Yang, Yukui Zhang, Bo Jiang,* Lihua Zhang* and Guangyan Qing*

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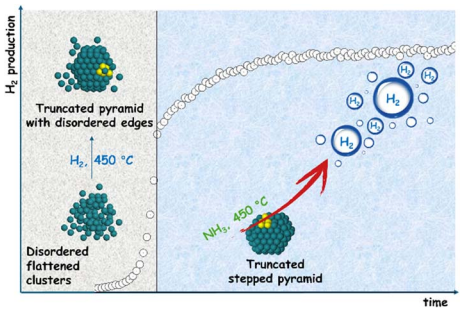
2648

Evolution of amorphous ruthenium nanoclusters into stepped truncated nano-pyramids on graphitic surfaces boosts hydrogen production from ammonia

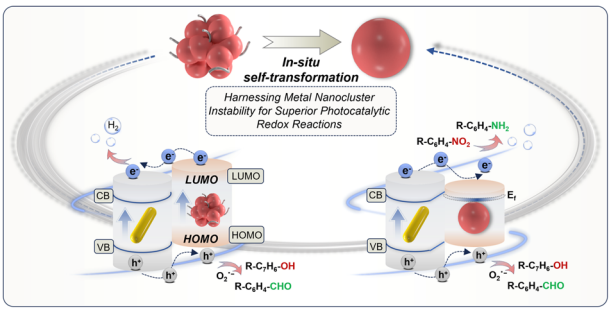
Yifan Chen, Benjamin J. Young, Gazi N. Aliev, Apostolos Kordatos, Ilya Popov, Sadegh Ghaderzadeh, Thomas J. Liddy, William J. Cull, Emerson C. Kohlrausch, Andreas Weilhard, Graham J. Hutchings, Elena Besley, Wolfgang Theis,* Jesum Alves Fernandes* and Andrei N. Khlobystov*



2661

Surmounting the instability of atomically precise metal nanoclusters towards boosted photoredox organic transformation

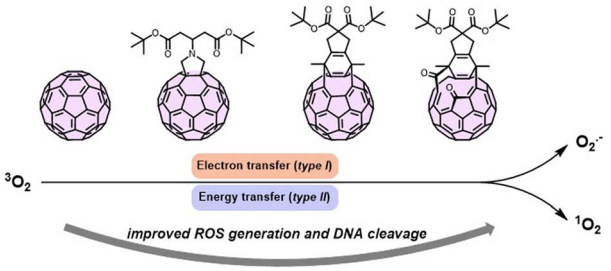
Yu-Bing Li and Fang-Xing Xiao*



2673

Enhancement of photoinduced reactive oxygen species generation in open-cage fullerenes

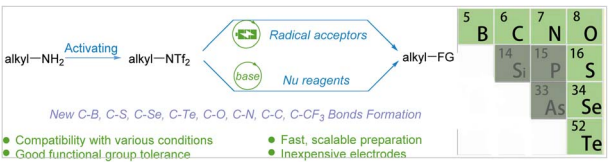
Cristina Castanyer, Çetin Çelik, Albert Artigas, Anna Roglans, Anna Pla-Quintana,* Anton J. Stasyuk,* Yoko Yamakoshi* and Miquel Solà*



2682

Alkyl bistriflimidate-mediated electrochemical deaminative functionalization

Hui Shu, Xiangzhang Tao,* Shengyang Ni, Jiyang Liu, Jia Xu, Yi Pan and Yi Wang*



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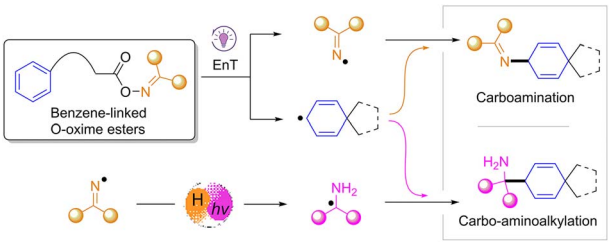
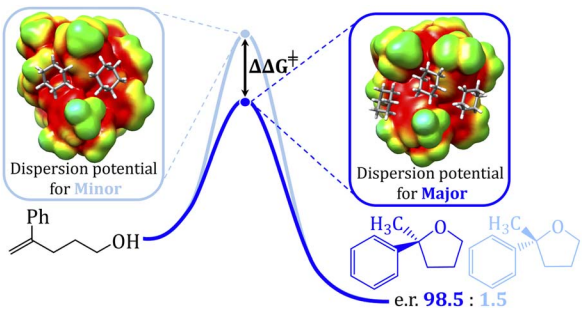


Chemodivergent dearomatization of benzene-linked O-oxime esters *via* EnT-induced radical cross-coupling

Guohui Zeng, Dongwen Guo, Huanfeng Jiang and Biaolin Yin*

2700



Understanding and quantifying the impact of solute–solvent van der Waals interactions on the selectivity of asymmetric catalytic transformations

Riya Kayal, Lorenzo Baldinelli, Ingolf Harden,* Frank Neese and Giovanni Bistoni*

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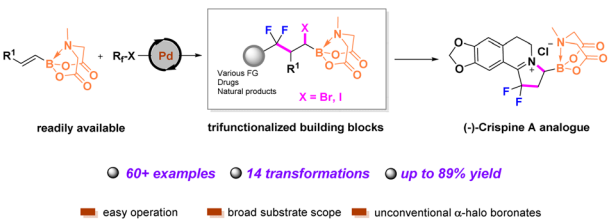

B(MIDA)-directed site-selective intermolecular halofluoroalkylation of alkenes: synthesis of diversely functionalized building blocks

Hengbo Wu, Ruitong Luo, Jingjing Peng, Zijian Han, Renjie Zhang, Zhijian Xu, Weiliang Zhu,* Hong Liu* and Chunpu Li*

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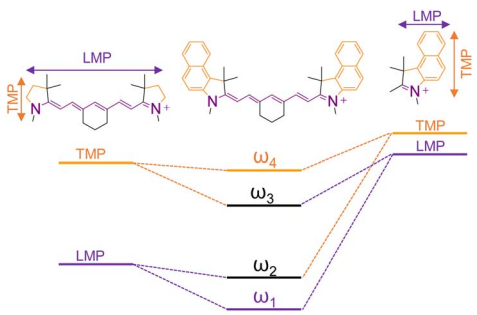

Plasmon hybridization model in molecules: molecular jackhammers

Ciceron Ayala-Orozco,* Bowen Li, Gang Li and James M. Tour*

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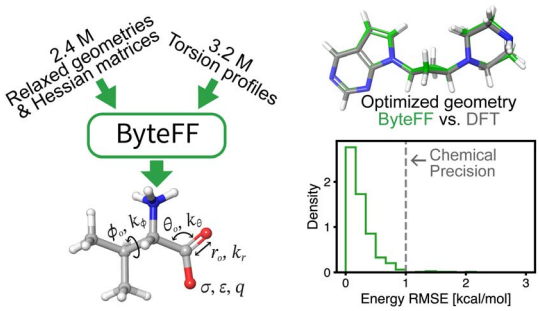
2730

Data-driven parametrization of molecular mechanics force fields for expansive chemical space coverage

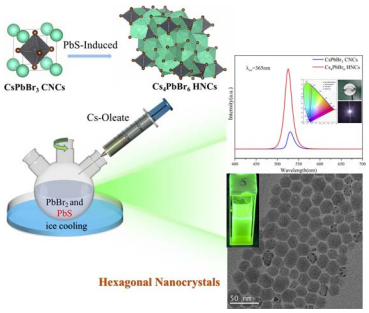
Tianze Zheng,* Ailun Wang, Xu Han, Yu Xia, Xingyuan Xu, Jiawei Zhan, Yu Liu, Yang Chen, Zhi Wang, Xiaojie Wu, Sheng Gong and Wen Yan*



2741

Influence of Lewis basicity on the S^{2-} induced synthesis of 0D Cs_4PbBr_6 hexagonal nanocrystals and its implications for optoelectronics

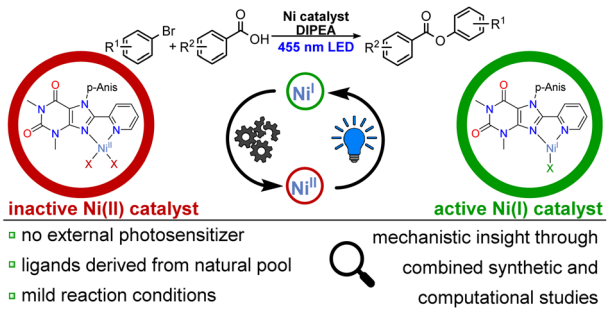
Yukun Liu, Yangai Liu,* Chenguang Yang, Lefu Mei, Hao Ding, Ruiyu Mi and Yuanyuan Zhang*



2751

Mechanistic insights into the visible-light-driven *O*-arylation of carboxylic acids catalyzed by xanthine-based nickel complexes

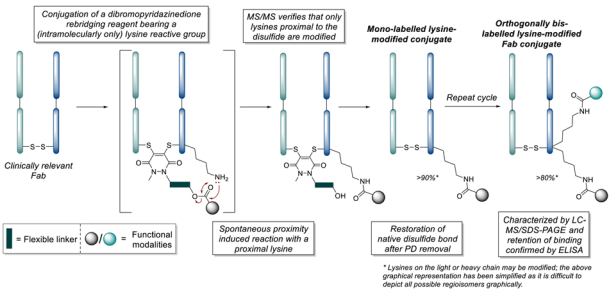
Rafael E. Rodriguez-Lugo,* Joan Sander, Simon Dietzmann, Thomas Rittner, Jannes Rückel, Vanessa R. Landaeta, Jiyong Park, Patrick Nuernberger, Mu-Hyun Baik* and Robert Wolf*



2763

Formation of mono- and dual-labelled antibody fragment conjugates *via* reversible site-selective disulfide modification and proximity induced lysine reactivity

Ioanna A. Thanasi, Nathalie Bouloc, Clíona McMahon, Ning Wang, Peter A. Szijj, Tobias Butcher, Léa N. C. Rochet, Elizabeth A. Love, Andy Merritt, James R. Baker* and Vijay Chudasama*



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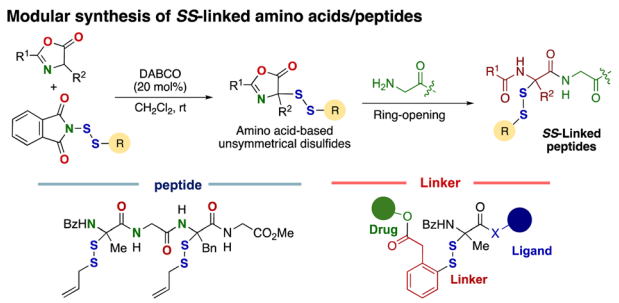
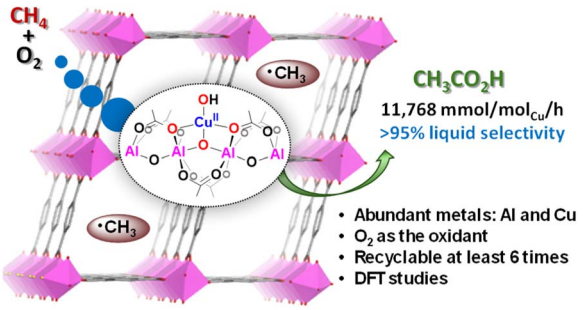


A versatile entry to unnatural, disulfide-linked amino acids and peptides through the disulfuration of azlactones

Masaki Iwata, Yuzuki Takami, Hayato Asanuma, Kenya Hosono, Hibiki Ohno, Naohiko Yoshikai and Kazuya Kanemoto*

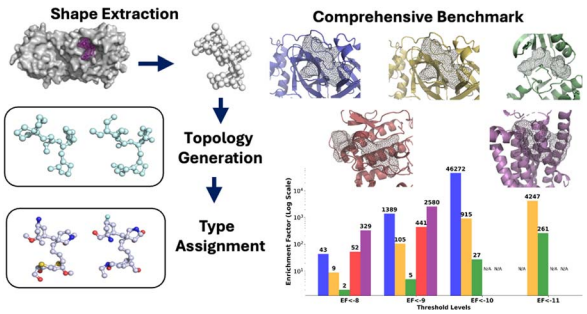
2785



Copper catalyzed selective methane oxidation to acetic acid using O_2

Poorvi Gupta, Bharti Rana, Rishabh Maurya, Rahul Kalita, Manav Chauhan and Kuntal Manna*

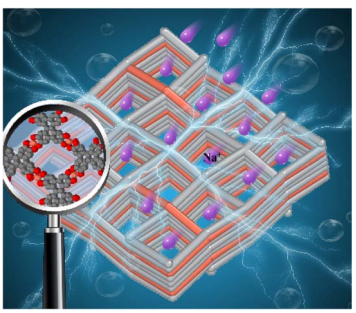
2796



TopMT-GAN: a 3D topology-driven generative model for efficient and diverse structure-based ligand design

Shen Wang, Tong Lin, Tianyi Peng, Enming Xing, Sijie Chen, Levent Burak Kara and Xiaolin Cheng*

2810



A 3D four-fold interpenetrated conductive metal–organic framework for fast and robust sodium-ion storage

Zhaoli Liu, Juan Chu, Linqi Cheng, Junhao Wang, Chongyi Zhang, Cheng Zhang, Fengchao Cui,* Heng-Guo Wang* and Guangshan Zhu

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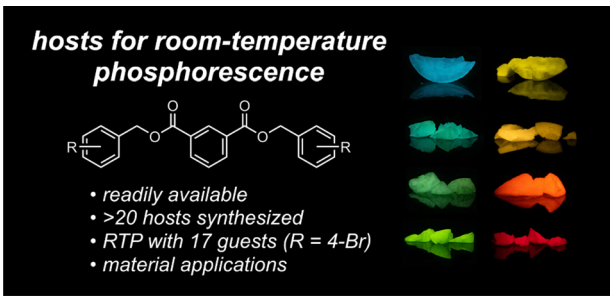
2819

Dibenzyl isophthalates as versatile hosts in room temperature phosphorescence host–guest systems

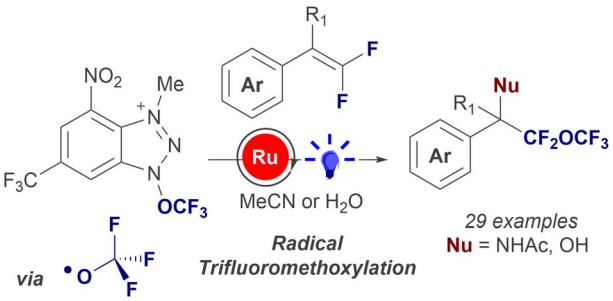
Martin Molkenthin, Emanuel Hupf* and Boris J. Nachtsheim*



2830

Radical trifluoromethoxylation of fluorinated alkenes for accessing difluoro(trifluoromethoxy) methyl groups

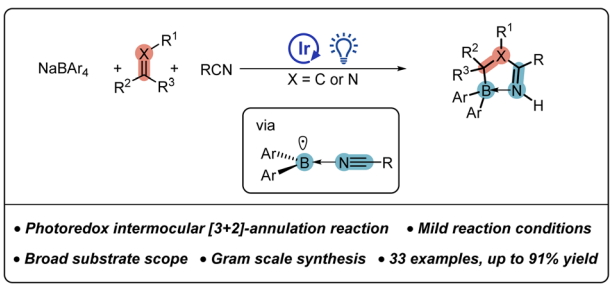
Koki Kawai, Mai Usui, Sota Ikawa, Naoyuki Hoshiya, Yosuke Kishikawa and Norio Shibata*



2837

Photocatalytic [3 + 2]-annulation *via* sodium tetraarylborate: a fundamental approach for synthesizing 1,4,2-diazaborole analogs

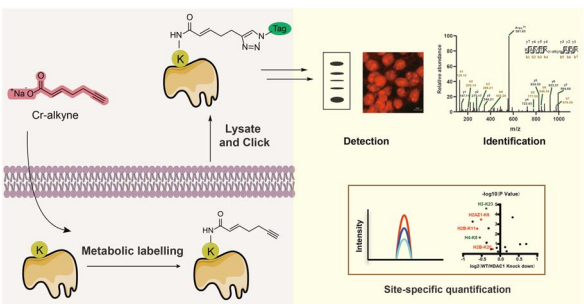
Hao-Ni Qin, Hao-Wen Jiang, Yi Zhao, Saira Qurban, Ke-Chun Wang and Peng-Fei Xu*



2843

Chemical proteomic profiling of lysine crotonylation using minimalist bioorthogonal probes in mammalian cells

Yuan-Fei Zhou, Shouli Yuan, Bin Ma, Jinjun Gao and Chu Wang*



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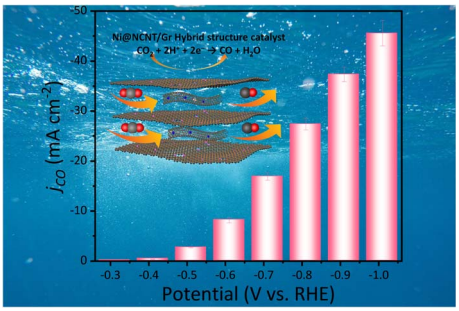
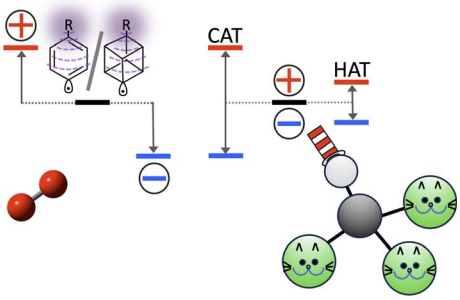


Design of a new Ni@NCNT/graphene hybrid structured catalyst for high-performance electrochemical CO_2 reduction: unravelling the roles of N-doping

Jian Zhu, Jing Hu, Zhenyu Wang, Zhouguang Lu, Shoubhik Das* and Pegie Cool*

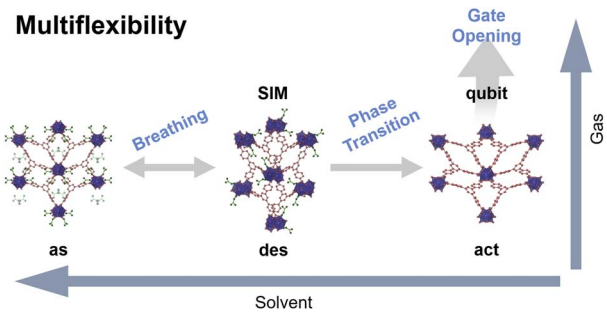
2861



Electrostatically tuning radical addition and atom abstraction reactions with distonic radical ions

Oisin J. Shiels, Samuel C. Brydon, Berwyck L. J. Poad, David L. Marshall, Sevan D. Houston, Hui Xing, Paul V. Bernhardt, G. Paul Savage, Craig M. Williams, David G. Harman, Benjamin B. Kirk, Gabriel da Silva, Stephen J. Blanksby* and Adam J. Trevitt*

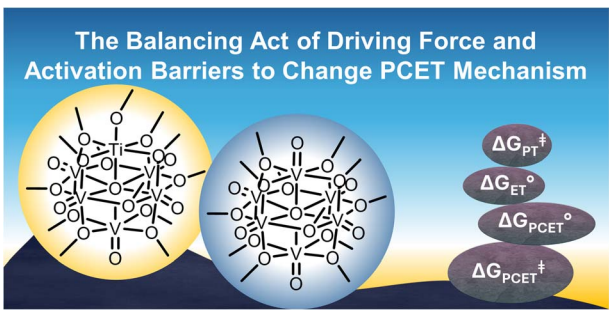
2879



Implementing magnetic properties on demand with a dynamic lanthanoid–organic framework

Iván Gómez-Muñoz, Ziqi Hu, Iñigo J. Vitórica-Yrezábal, Eugenio Coronado and Guillermo Mínguez Espallargas*

2886



Engineering mechanisms of proton-coupled electron transfer to a titanium-substituted polyoxovanadate–alkoxide

Shannon E. Cooney, S. Genevieve Duggan, M. Rebecca A. Walls, Noah J. Gibson, James M. Mayer, Pere Miro* and Ellen M. Matson*

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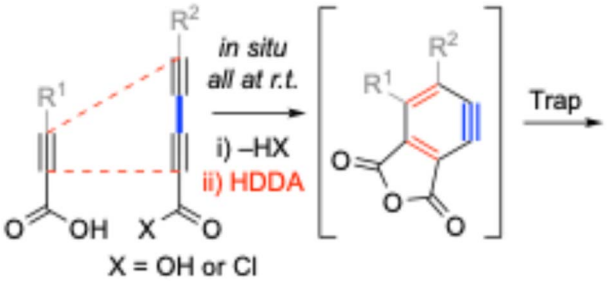
EDGE ARTICLES

2898

Rapid (≤25 °C) cycloisomerization of anhydride-tethered triynes to benzynes – origin of a remarkable anhydride linker-induced rate enhancement

Dorian S. Sneddon, Paul V. Kevorkian and Thomas R. Hoye*



2907

Grappa – a machine learned molecular mechanics force field

Leif Seute,* Eric Hartmann, Jan Stühmer and Frauke Gräter*

CORRECTION

2931

Correction: Strategic design of GalNAc-helical peptide ligands for efficient liver targeting

Takahito Ito, Nobumichi Ohoka, Michihiko Aoyama, Takashi Nishikaze, Takashi Misawa, Takao Inoue, Akiko Ishii-Watabe and Yosuke Demizu*