

IN THIS ISSUE

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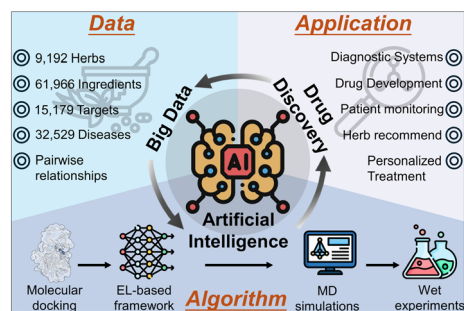
Inside cover
See Jana Selent, Mette Marie Rosenkilde *et al.*, pp. 10671–10683. Image reproduced by permission of Viktoria Madeline Skovgaard Kjær, Tomasz Stepniewski, Mette Rosenkilde and Jana Selent from *Chem. Sci.*, 2023, 14, 10671.

COMMENTARY

10628

A focus on harnessing big data and artificial intelligence: revolutionizing drug discovery from traditional Chinese medicine sources

Mingyu Li and Jian Zhang*

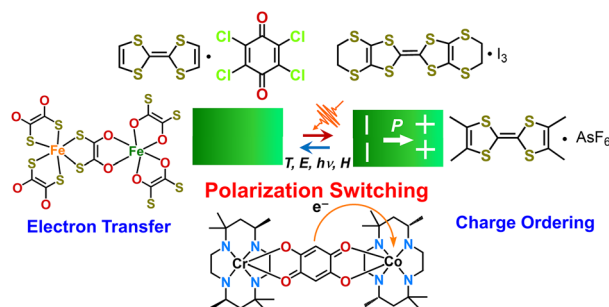


PERSPECTIVES

10631

Control of electronic polarization *via* charge ordering and electron transfer: electronic ferroelectrics and electronic pyroelectrics

Sheng-Qun Su, Shu-Qi Wu, Shinji Kanegawa, Kaoru Yamamoto and Osamu Sato*



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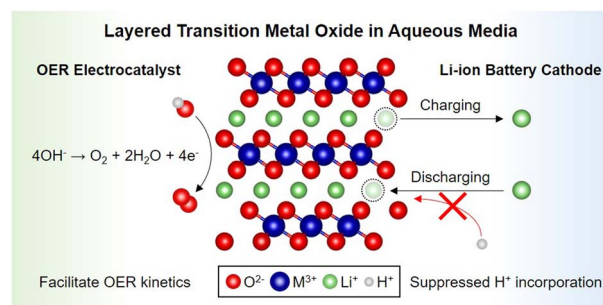


PERSPECTIVES

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Layered transition metal oxides (LTMO) for oxygen evolution reactions and aqueous Li-ion batteries

Yohan Kim, Eunjin Choi, Seunggu Kim and Hye Ryung Byon*

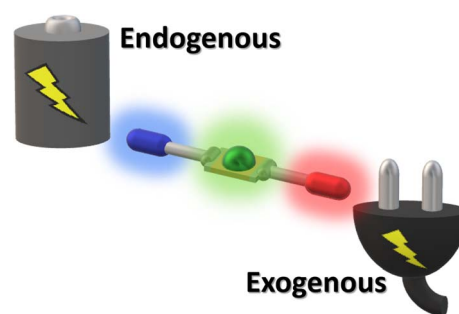


EDGE ARTICLES

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Endogenous and exogenous wireless multimodal light-emitting chemical devices

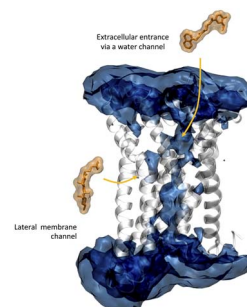
Miaoxia Liu, Gerardo Salinas, Jing Yu, Antoine Cornet, Haidong Li, Alexander Kuhn* and Neso Sojic*



10671

Ligand entry pathways control the chemical space recognized by GPR183

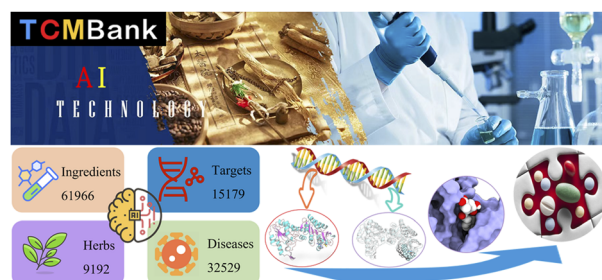
Viktoria Madeline Skovgaard Kjær, Tomasz Maciej Stępniewski, Brian Medel-Lacruz, Lisa Reinmuth, Marija Ciba, Elisabeth Rexen Ulven, Massimiliano Bonomi, Jana Selent* and Mette Marie Rosenkilde*



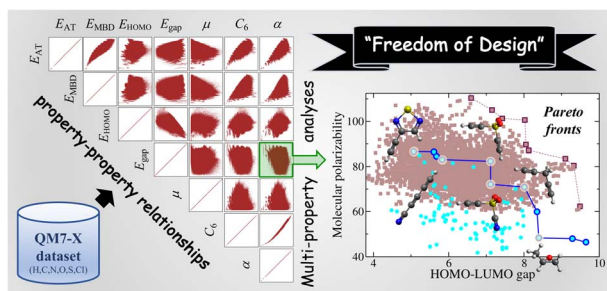
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TCMBank: bridges between the largest herbal medicines, chemical ingredients, target proteins, and associated diseases with intelligence text mining

Qiujie Lv, Guanxing Chen, Haohuai He, Ziduo Yang, Lu Zhao, Hsin-Yi Chen and Calvin Yu-Chian Chen*



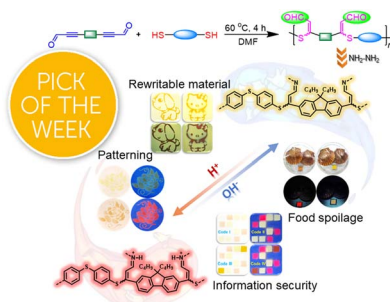
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“Freedom of design” in chemical compound space: towards rational *in silico* design of molecules with targeted quantum-mechanical properties

Leonardo Medrano Sandonas,^{*} Johannes Hoja, Brian G. Ernst, Álvaro Vázquez-Mayagoitia, Robert A. DiStasio, Jr.^{*} and Alexandre Tkatchenko^{*}

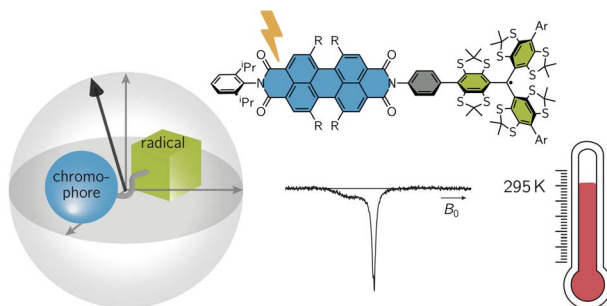
10718



Acid–base responsive multifunctional poly(formyl sulfide)s through a facile catalyst-free click polymerization of aldehyde-activated internal diynes and dithiols

Baixue Li, Xue Wang, Die Huang, Mingzhao Li, Anjun Qin,^{*} Yusheng Qin^{*} and Ben Zhong Tang

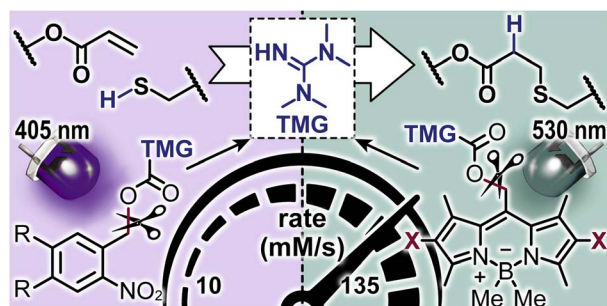
10727



PDI–trityl dyads as photogenerated molecular spin qubit candidates

Maximilian Mayländer, Kevin Kopp, Oliver Nolden, Michael Franz, Philipp Thielert, Andreas Vargas Jentzsch, Peter Gilch, Olav Schiemann and Sabine Richert^{*}

10736



Record release of tetramethylguanidine using a green light activated photocage for rapid synthesis of soft materials

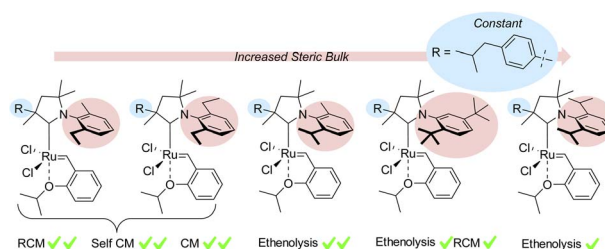
Kun-You Chung, Ain Uddin and Zachariah A. Page^{*}



10744

A tunable family of CAAC-ruthenium olefin metathesis catalysts modularly derived from a large-scale produced ibuprofen intermediate

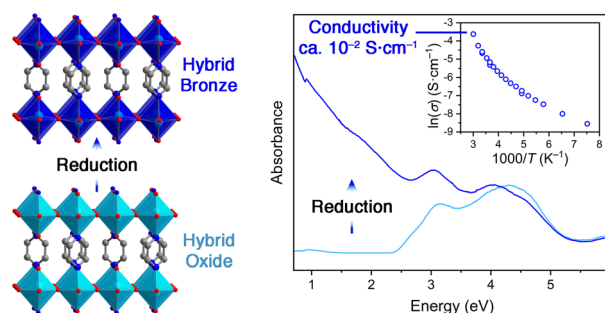
Adrian Sytniczuk, Filip Struzik, Karol Grela and Anna Kajetanowicz*



10756

Hybrid bronzes: mixed-valence organic–inorganic metal oxides as a tunable material platform

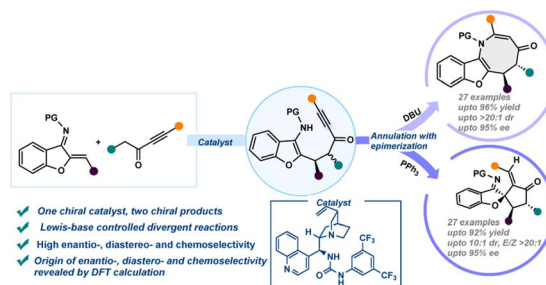
W. Lakna N. Dayaratne, Raúl Torres-Cadena, Bennett P. Schmitt, Emma M. Westrick and Adam Jaffe*



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Structurally divergent enantioselective synthesis of benzofuran fused azocine derivatives and spirocyclopentanone benzofurans enabled by sequential catalysis

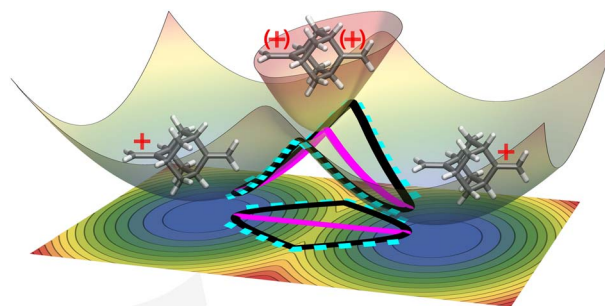
Rupkumar Khuntia, Sanat Kumar Mahapatra, Lisa Roy and Subhas Chandra Pan*



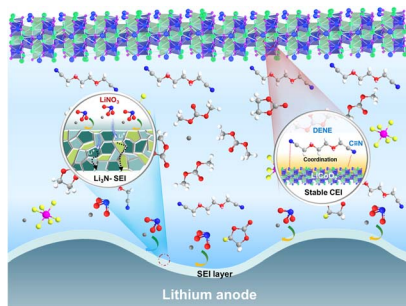
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Competing quantum effects in heavy-atom tunnelling through conical intersections

Wei Fang, Eric R. Heller and Jeremy O. Richardson*



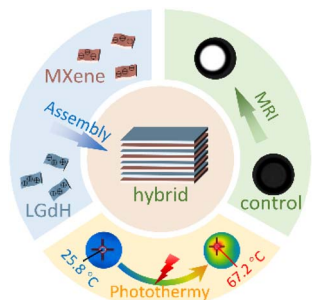
10786



High-voltage lithium-metal batteries enabled by ethylene glycol bis(propionitrile) ether-LiNO₃ synergistic additives

Shaopeng Li, Kangsheng Huang, Langyuan Wu, Dewei Xiao, Jiang Long, Chenhui Wang, Hui Dou, Pu Chen* and Xiaogang Zhang*

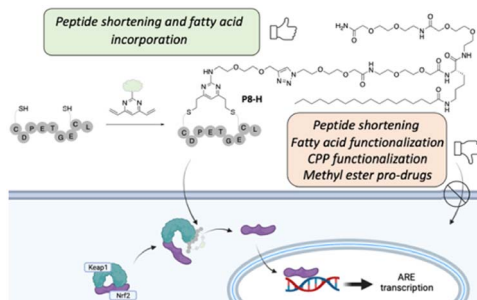
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Rare-earth hydroxide/MXene hybrid: a promising agent for near-infrared phototherapy and magnetic resonance imaging

Mingjun Bai, Linawati Sutrisno, Junhong Duan, Hao Wan,* Gen Chen, Xiaohe Liu* and Renzhi Ma*

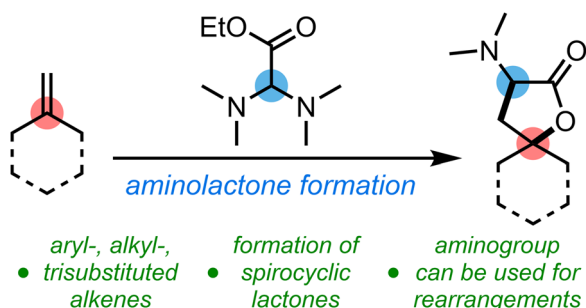
10800



A cell-active cyclic peptide targeting the Nrf2/Keap1 protein-protein interaction

Jessica Iegre, Sona Krajcovicova, Anders Gunnarsson, Lisa Wissler, Helena Käck, Anna Luchniak, Stefan Tångebjerg, Frank Narjes* and David R. Spring*

10806



General acid-mediated aminolactone formation using unactivated alkenes

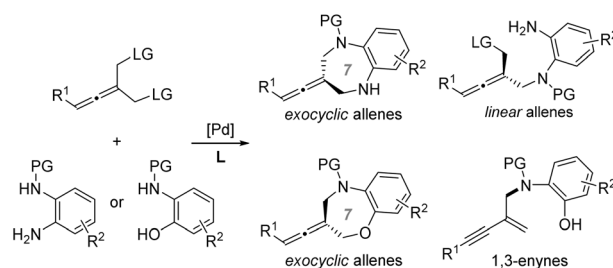
David Just, Carlos R. Gonçalves, Uroš Vezonik, Daniel Kaiser and Nuno Maulide*



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Chemodivergence in Pd-catalyzed desymmetrization of allenes: enantioselective [4+3] cycloaddition, desymmetric allenylic substitution and enynylation

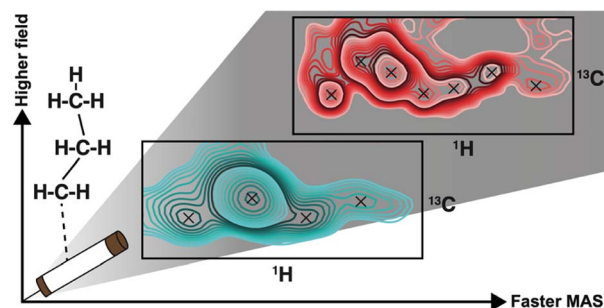
Pengfei Luo, Long Li, Xinfang Mao, Zheng Sun, Yingcheng Wang, Fangzhi Peng and Zhihui Shao*



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High and fast: NMR protein–proton side-chain assignments at 160 kHz and 1.2 GHz

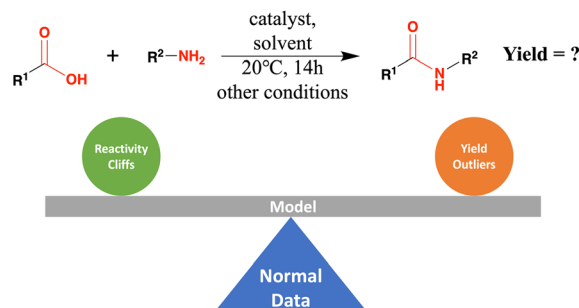
Morgane Callon,* Dominique Luder, Alexander A. Malär, Thomas Wiegand, Václav Římal, Lauriane Lecoq, Anja Böckmann, Ago Samoson and Beat H. Meier*



10835

The challenge of balancing model sensitivity and robustness in predicting yields: a benchmarking study of amide coupling reactions

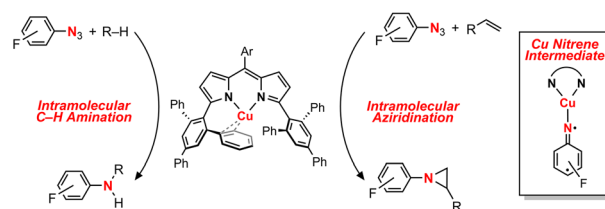
Zhen Liu, Yurii S. Moroz and Olexandr Isayev*



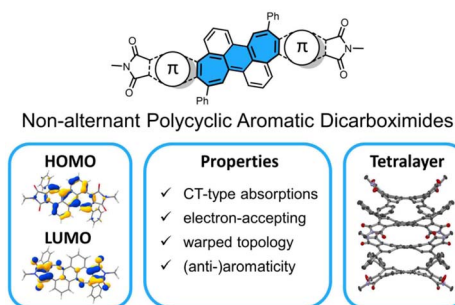
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Nitrene transfer from a sterically confined copper nitrenoid dipyrin complex

Kurtis M. Carsch, Sasha C. North, Ida M. DiMucci, Andrei Iliescu, Petra Vojáčková, Thomas Khazanov, Shao-Liang Zheng, Thomas R. Cundari, Kyle M. Lancaster and Theodore A. Betley*



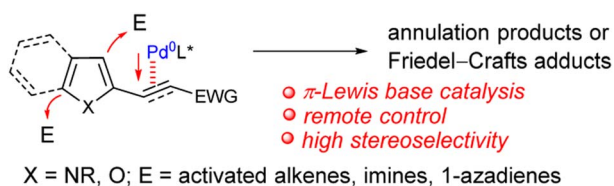
10861



π -Extended benzo[1,2:4,5]di[7]annulene bis(dicarboximide)s – a new class of non-alternant polycyclic aromatic dicarboximides

Jonas Spengler, Chongwei Zhu, Kazutaka Shoyama and Frank Würthner*

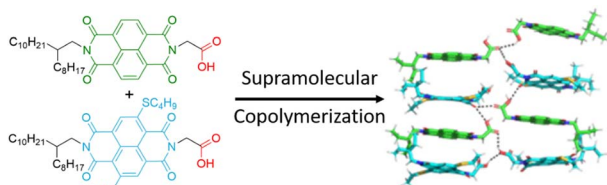
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Asymmetric Friedel–Crafts reaction of unsaturated carbonyl-tethered heteroarenes via vinylogous activation of Pd⁰– π -Lewis base catalysis

Bo Jiang, Wu-Tao Gui, Hao-Tian Wang, Ke Xie, Zhi-Chao Chen, Lei Zhu, Qin Ouyang,* Wei Du* and Ying-Chun Chen*

10875



Supramolecular alternating copolymers with highly efficient fluorescence resonance energy transfer

Anwasha Chakraborty, Pradipta Kumar Das, Biman Jana* and Suhrit Ghosh*

10884

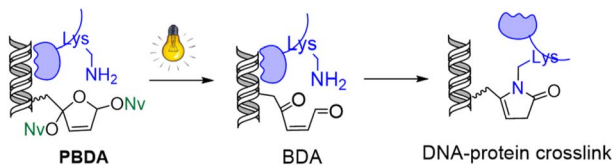


Photo-caged 2-butene-1,4-dial as an efficient, target-specific photo-crosslinker for covalent trapping of DNA-binding proteins

Jiahui Li, Zenghui Cui, Chaochao Fan, Yifei Zhou, Mengtian Ren and Chuangzheng Zhou*

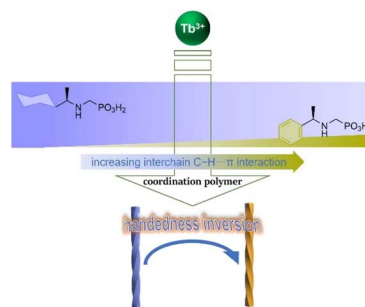
- High specificity for DNA-binding proteins (Lys-rich)
- High photo-crosslinking yields (70%) in minutes



10892

Macroscopic handedness inversion of terbium coordination polymers achieved by doping homochiral ligand analogues

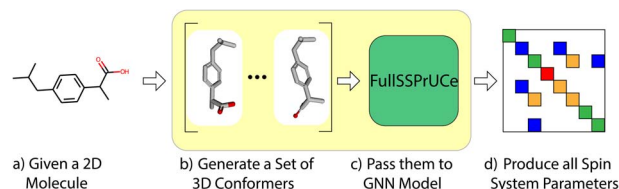
Chang-Yu Wang, Jia-Ge Jia, Guo-Guo Weng, Ming-Feng Qin, Kui Xu and Li-Min Zheng*



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Rapid prediction of full spin systems using uncertainty-aware machine learning

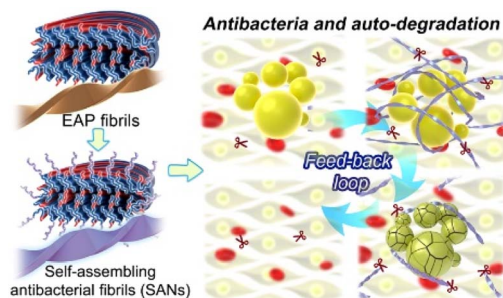
Jake Williams* and Eric Jonas



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Engineering of antimicrobial peptide fibrils with feedback degradation of bacterial-secreted enzymes

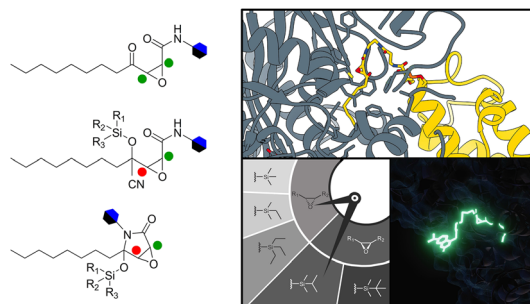
Fenghua Wang, Wencheng Xia, Mingming Zhang, Rongrong Wu, Xiaolu Song, Yun Hao, Yonghai Feng, Liwei Zhang, Dan Li, Wenyan Kang, Cong Liu* and Lei Liu*



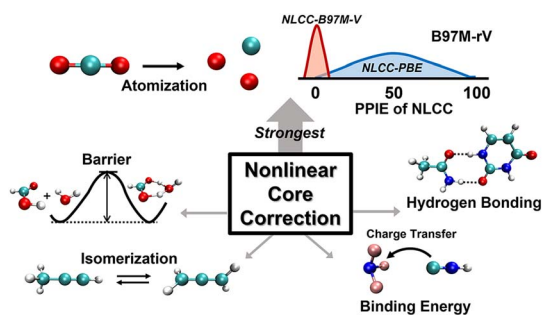
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Masked cerulenin enables a dual-site selective protein crosslink

Ziran Jiang, Aochiu Chen, Jeffrey Chen, Arman Sekhon, Gordon V. Louie, Joseph P. Noel, James J. La Clair and Michael D. Burkart*



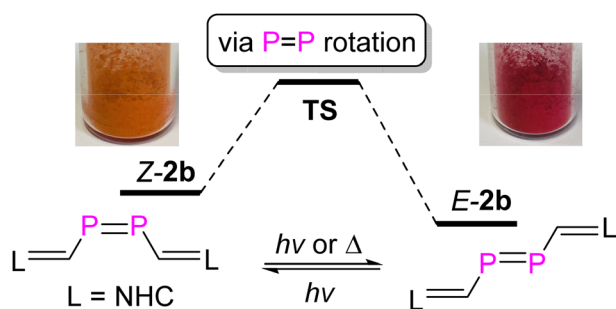
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Greater transferability and accuracy of norm-conserving pseudopotentials using nonlinear core corrections

Wan-Lu Li, Kaixuan Chen, Elliot Rossomme, Martin Head-Gordon and Teresa Head-Gordon*

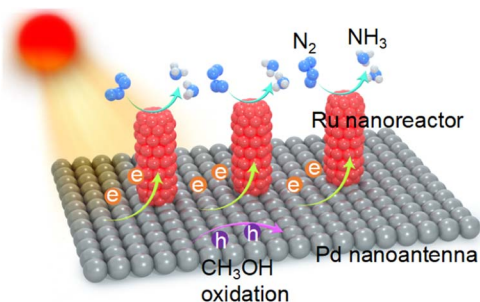
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Room temperature stable *E,Z*-diphosphenes: their isomerization, coordination, and cycloaddition chemistry

Jieli Lin, Shihua Liu, Jie Zhang, Hansjörg Grützmacher, Cheng-Yong Su and Zhongshu Li*

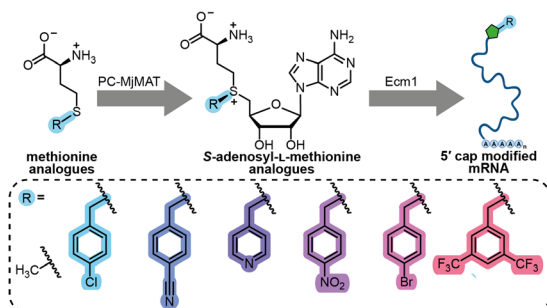
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A Pd-based plasmonic photocatalyst for nitrogen fixation through an antenna–reactor mechanism

Yuanyuan Yang, Henglei Jia,* Sihua Su, Yidi Zhang, Mengxuan Zhao, Jingzhao Li, Qifeng Ruan* and Chun-yang Zhang*

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Post-synthetic benzylation of the mRNA 5' cap via enzymatic cascade reactions

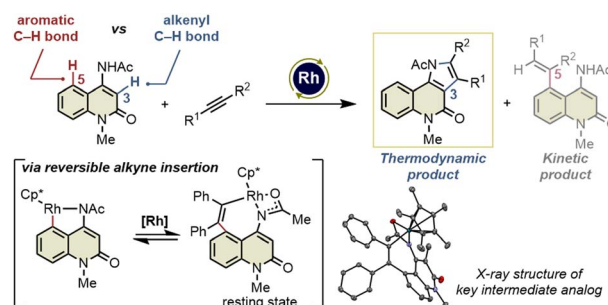
N. V. Cornelissen, R. Mineikaitė, M. Erguven, N. Muthmann, A. Peters, A. Bartels and A. Rentmeister*



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Rh(III)-catalyzed highly site- and regio-selective alkenyl C–H activation/annulation of 4-amino-2-quinolones with alkynes *via* reversible alkyne insertion

Naohiro Hirako, Takeshi Yasui* and Yoshihiko Yamamoto*



CORRECTION

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Correction: Improving time-resolution and sensitivity of *in situ* X-ray photoelectron spectroscopy of a powder catalyst by modulated excitation

M. Roger, L. Artiglia,* A. Boucly, F. Buttignol, M. Agote-Arán, J. A. van Bokhoven, O. Kröcher and D. Ferri*

