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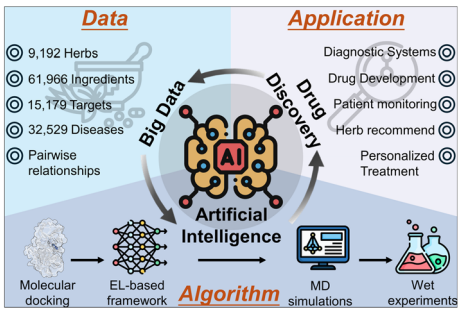
Inside cover
See Jana Selent, Mette Marie Rosenkilde *et al.*, pp. 10671–10683. Image reproduced by permission of Viktoria Madeline Skovgaard Kjær, Tomasz Stepniewski, Mette Rosenkilde and Jana Selent from *Chem. Sci.*, 2023, **14**, 10671.

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

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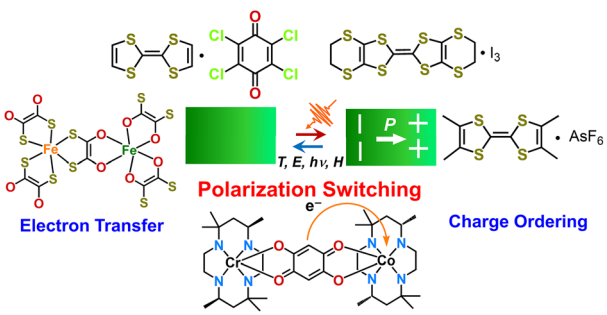
Control of electronic polarization *via* charge ordering and electron transfer: electronic ferroelectrics and electronic pyroelectrics

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



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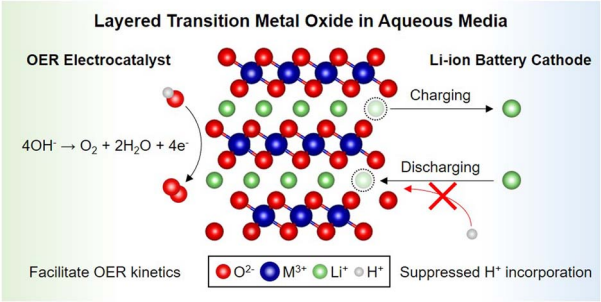
Layered transition metal oxides (LTMO) for oxygen evolution reactions and aqueous Li-ion batteries

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



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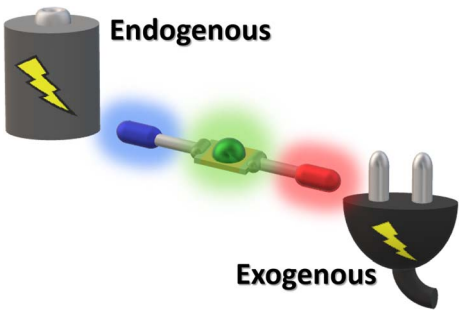
Endogenous and exogenous wireless multimodal light-emitting chemical devices

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



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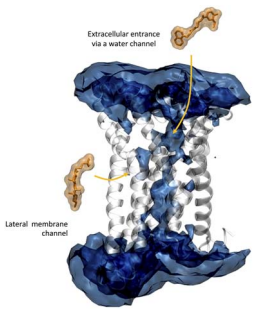
Ligand entry pathways control the chemical space recognized by GPR183

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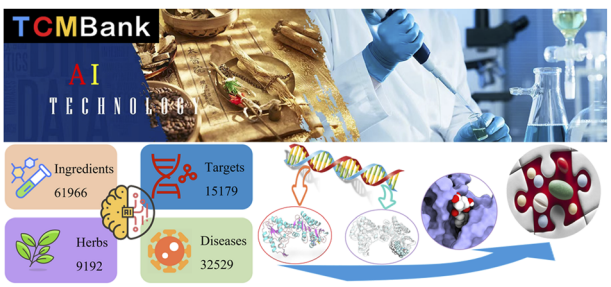
TCMBank: bridges between the largest herbal medicines, chemical ingredients, target proteins, and associated diseases with intelligence text mining

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



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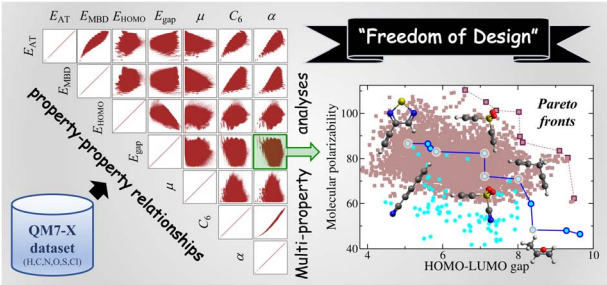

"Freedom of design" in chemical compound space: towards rational *in silico* design of molecules with targeted quantum-mechanical properties

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

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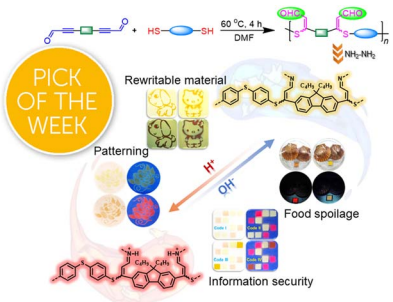

Acid–base responsive multifunctional poly(formyl sulfide)s through a facile catalyst-free click polymerization of aldehyde-activated internal diynes and dithiols

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

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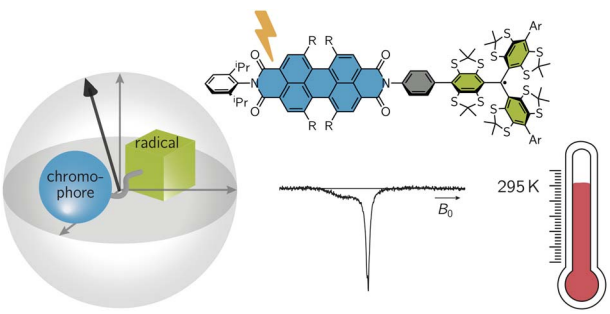

PDI–trityl dyads as photogenerated molecular spin qubit candidates

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

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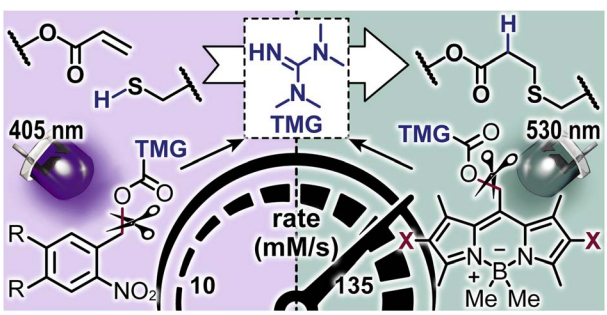

Record release of tetramethylguanidine using a green light activated photocage for rapid synthesis of soft materials

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

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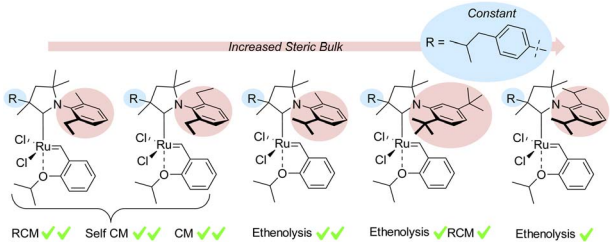
A tunable family of CAAC-ruthenium olefin metathesis catalysts modularly derived from a large-scale produced ibuprofen intermediate

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



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

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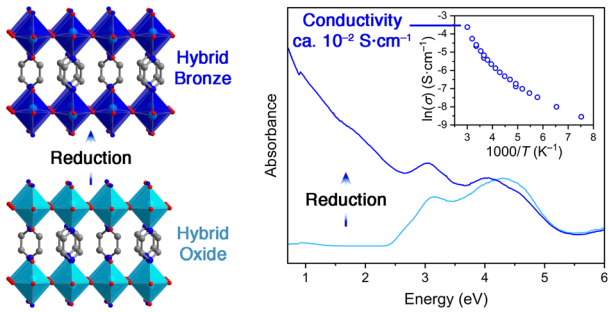

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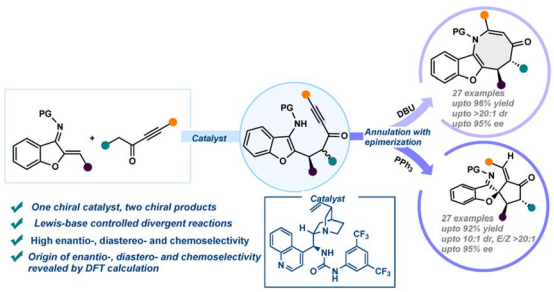
Structurally divergent enantioselective synthesis of benzofuran fused azocine derivatives and spiro-cyclopentanone benzofurans enabled by sequential catalysis

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

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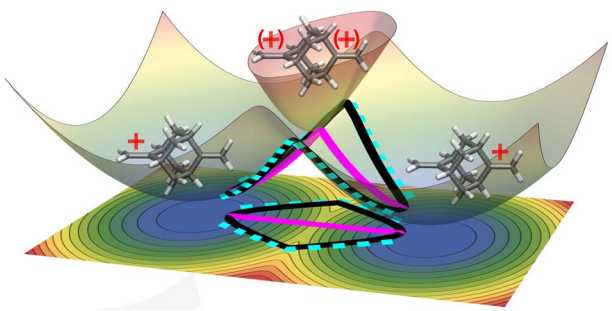

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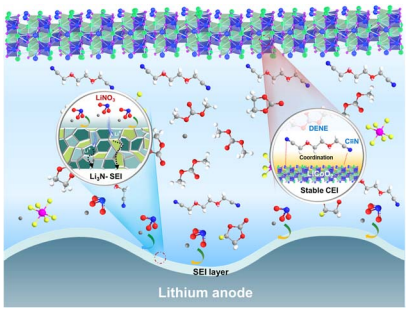

High-voltage lithium-metal batteries enabled by ethylene glycol bis(propionitrile) ether-$LiNO_3$ synergetic additives

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

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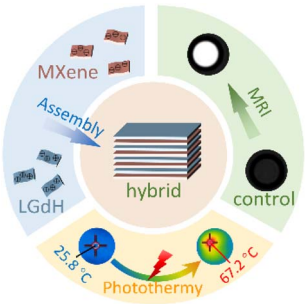

Rare-earth hydroxide/MXene hybrid: a promising agent for near-infrared photothermy and magnetic resonance imaging

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

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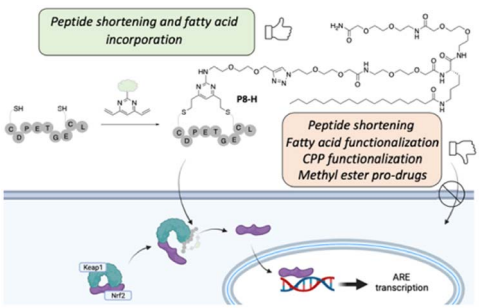

A cell-active cyclic peptide targeting the Nrf2/Keap1 protein–protein interaction

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

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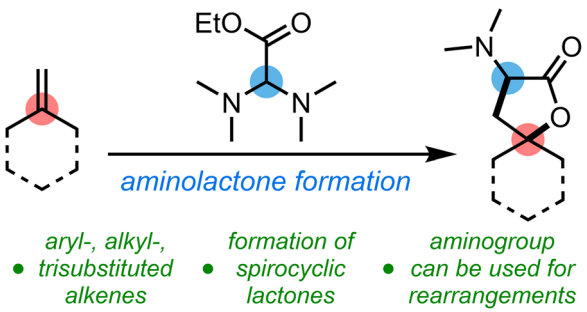

General acid-mediated aminolactone formation using unactivated alkenes

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

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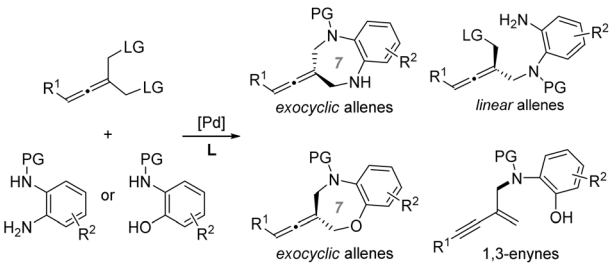
Chemodivergence in Pd-catalyzed desymmetrization of allenes: enantioselective [4+3] cycloaddition, desymmetric allenylic substitution and enynylation

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



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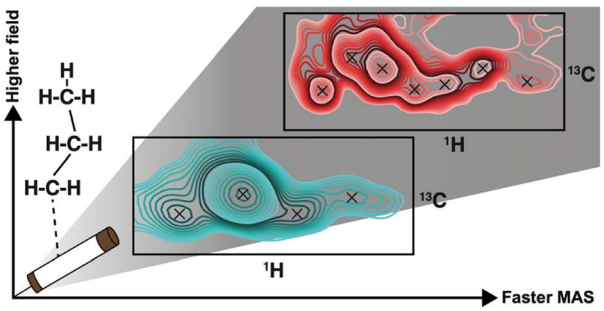
High and fast: NMR protein–proton side-chain assignments at 160 kHz and 1.2 GHz

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



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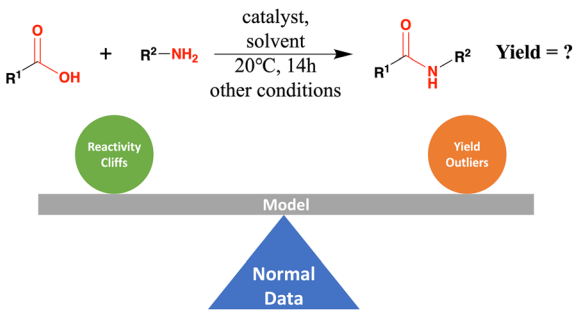
The challenge of balancing model sensitivity and robustness in predicting yields: a benchmarking study of amide coupling reactions

Zhen Liu, Yurii S. Moroz and Olexandr Isayev*



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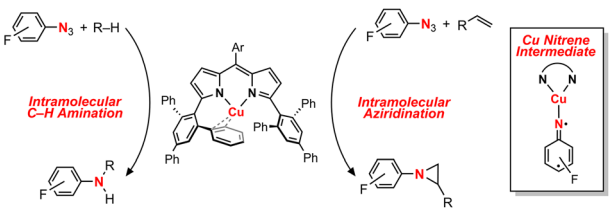
Nitrene transfer from a sterically confined copper nitrenoid dipyrrin complex

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*



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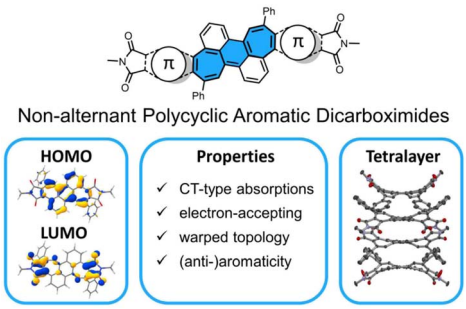
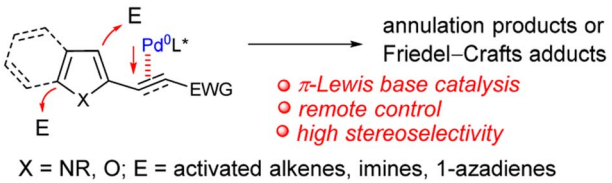


π-Extended benzo[1,2:4,5]di[7]annulene bis(dicarboximide)s – a new class of non-alternant polycyclic aromatic dicarboximides

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

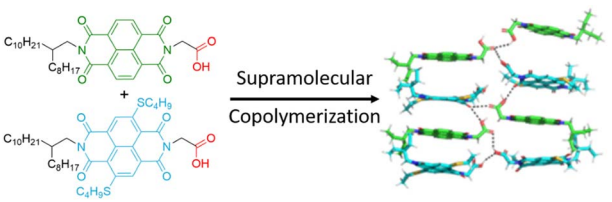
10867



Asymmetric Friedel–Crafts reaction of unsaturated carbonyl-tethered heteroarenes *via* vinylogous activation of Pd^0-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

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

10884

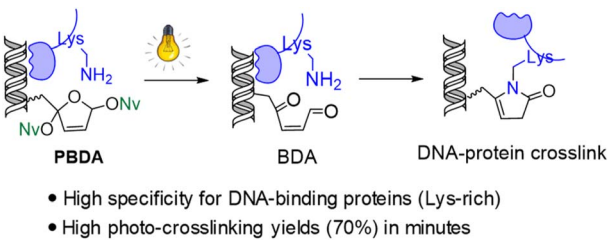


Photo-caged 2-butene-1,4-dial as an efficient, target-specific photo-crosslinker for covalent trapping of DNA-binding proteins

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

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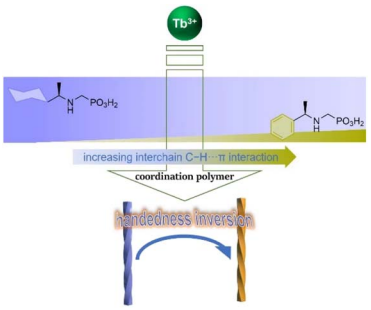
10892

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

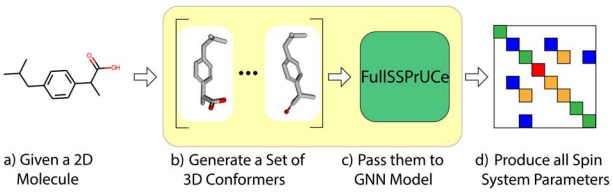
Chang-Yu Wang, Jia-Ge Jia, Guo-Guo Weng, Ming-Feng Qin, Kui Xu and Li-Min Zheng*



10902

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

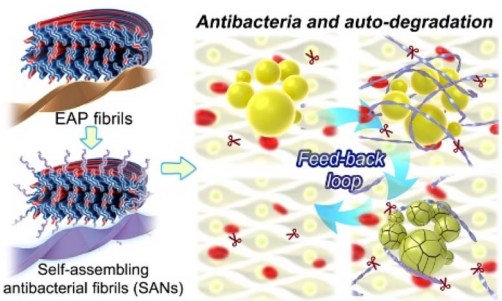
Jake Williams* and Eric Jonas



10914

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

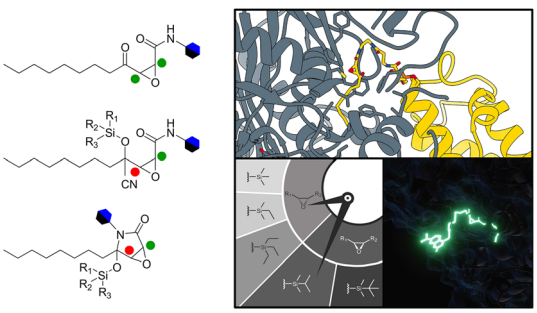
Fenghua Wang, Wencheng Xia, Mingming Zhang, Rongrong Wu, Xiaolu Song, Yun Hao, Yonghai Feng, Liwei Zhang, Dan Li, Wenyan Kang, Cong Liu* and Lei Liu*



10925

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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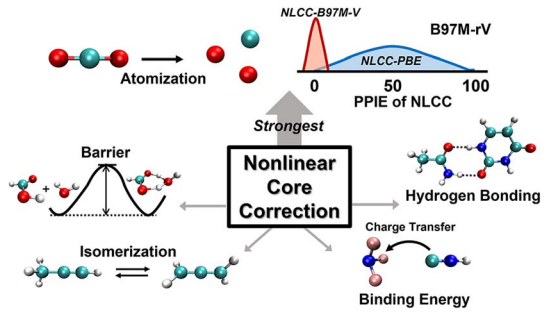
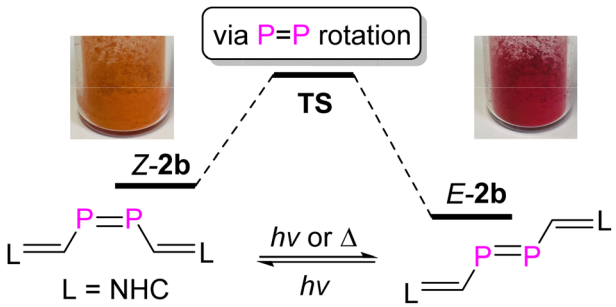
10934



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*

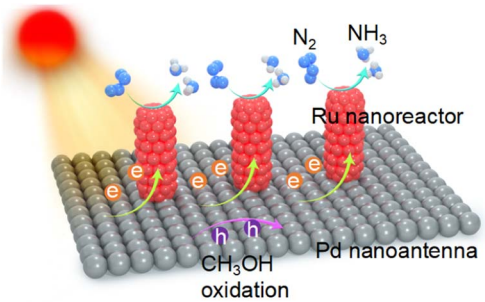
10944



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*

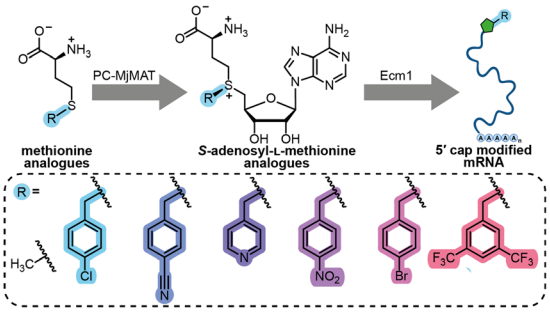
10953



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*

10962



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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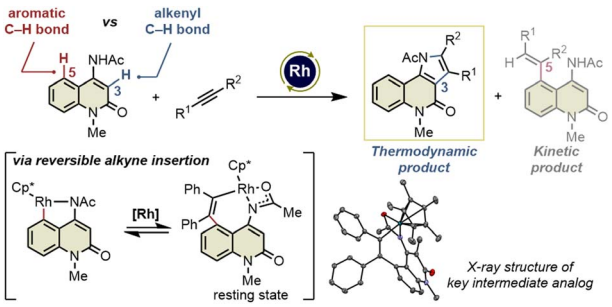
10971

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

10979

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*