

## IN THIS ISSUE

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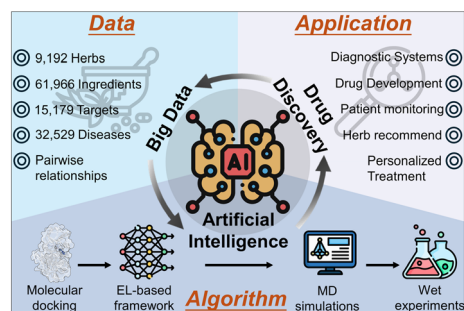
**Inside cover**  
See Jana Selent, Mette Marie Rosenkilde *et al.*, pp. 10671–10683. Image reproduced by permission of Viktoria Madeline Skovgaard Kjær, Tomasz Stepniewski, Mette Rosenkilde and Jana Selent from *Chem. Sci.*, 2023, 14, 10671.

## COMMENTARY

10628

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

Mingyu Li and Jian Zhang\*

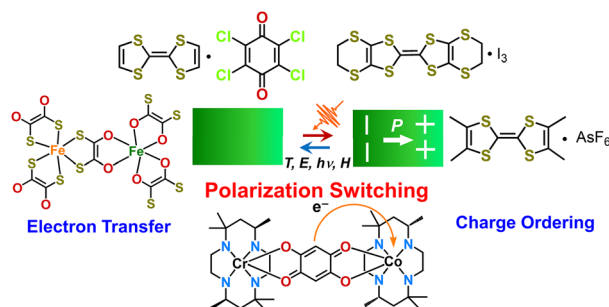


## PERSPECTIVES

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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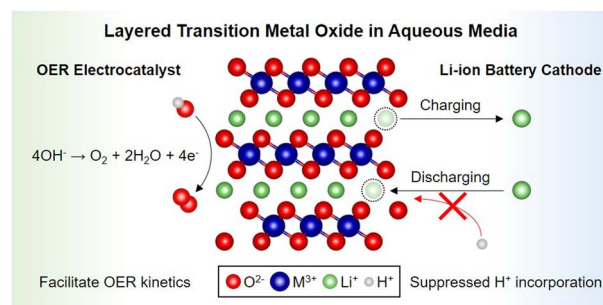


## PERSPECTIVES

10644

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

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

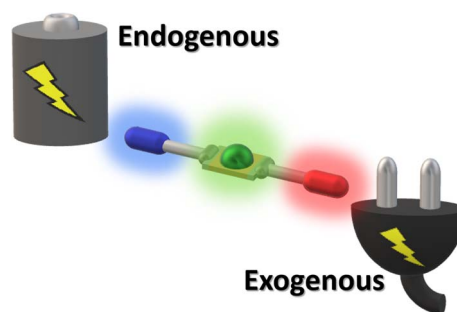


## EDGE ARTICLES

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**Endogenous and exogenous wireless multimodal light-emitting chemical devices**

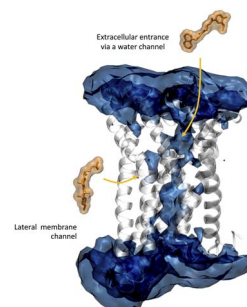
Miaoxia Liu, Gerardo Salinas, Jing Yu, Antoine Cornet, Haidong Li, Alexander Kuhn\* and Neso Sojic\*



10671

**Ligand entry pathways control the chemical space recognized by GPR183**

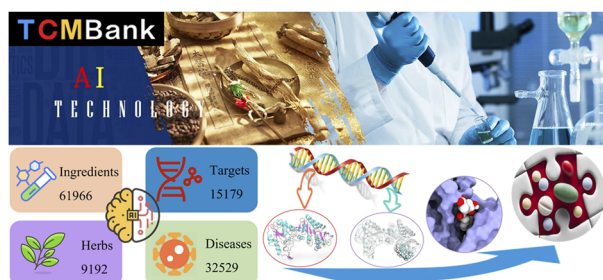
Viktoria Madeline Skovgaard Kjær, Tomasz Maciej Stępniewski, Brian Medel-Lacruz, Lisa Reinmuth, Marija Ciba, Elisabeth Rexen Ulven, Massimiliano Bonomi, Jana Selent\* and Mette Marie Rosenkilde\*



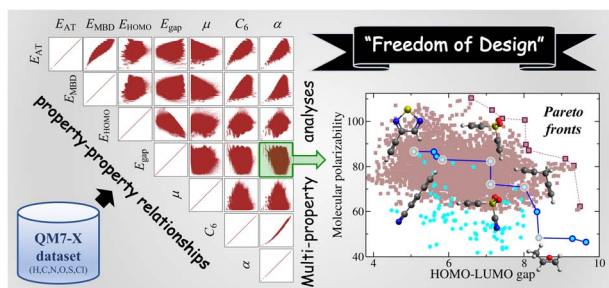
10684

**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\*



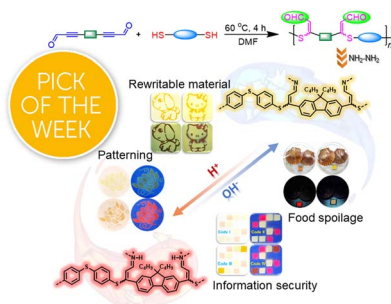
10702



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

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

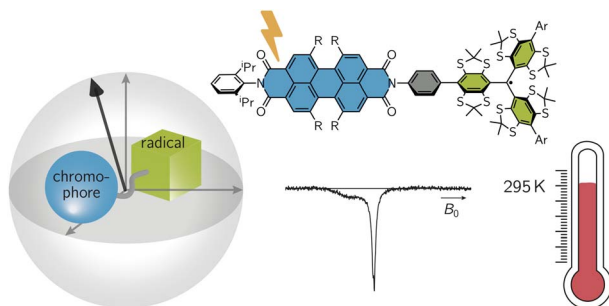
10718



### 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,<sup>\*</sup> Yusheng Qin<sup>\*</sup> and Ben Zhong Tang

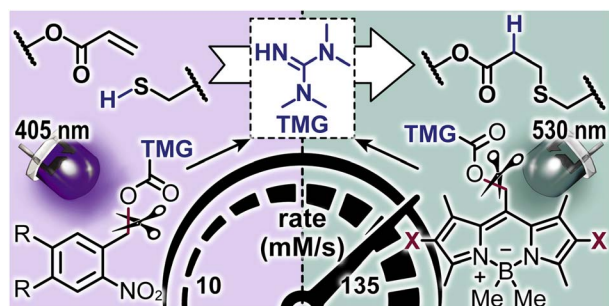
10727



### 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<sup>\*</sup>

10736



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

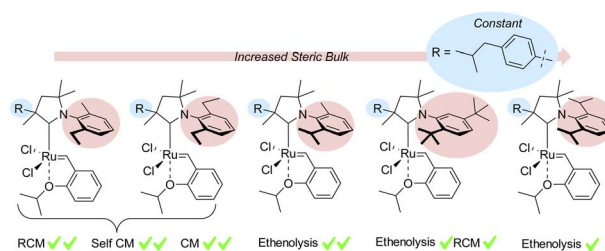
Kun-You Chung, Ain Uddin and Zachariah A. Page<sup>\*</sup>



10744

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

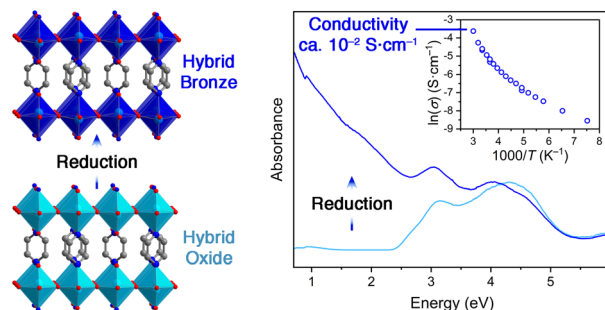
Adrian Sytniczuk, Filip Struzik, Karol Grela and Anna Kajetanowicz\*



10756

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

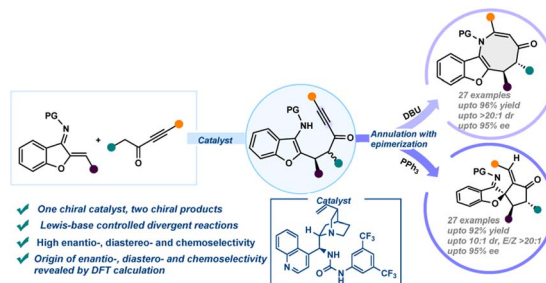
W. Lakna N. Dayaratne, Raúl Torres-Cadena, Bennett P. Schmitt, Emma M. Westrick and Adam Jaffe\*



10768

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

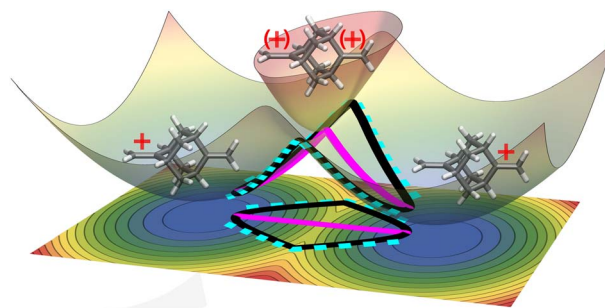
Rupkumar Khuntia, Sanat Kumar Mahapatra, Lisa Roy and Subhas Chandra Pan\*



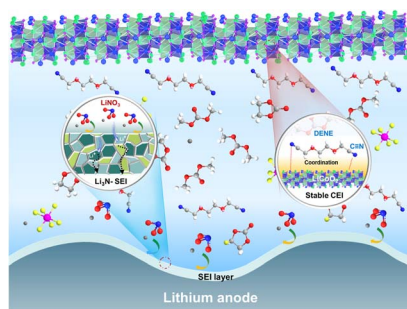
10777

## Competing quantum effects in heavy-atom tunnelling through conical intersections

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



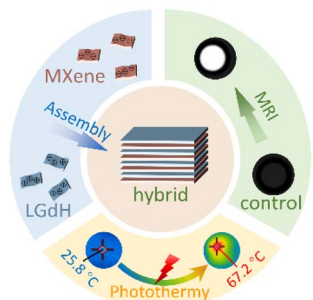
10786



### High-voltage lithium-metal batteries enabled by ethylene glycol bis(propionitrile) ether-LiNO<sub>3</sub> synergistic additives

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

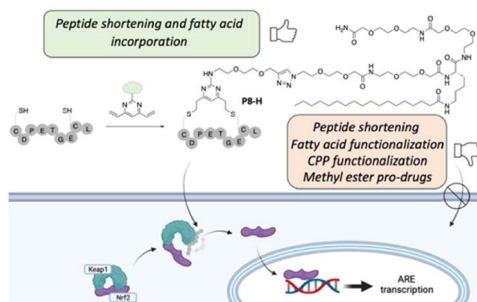
10795



### 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\*

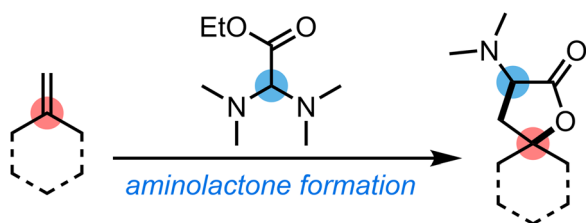
10800



### 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



- aryl-, alkyl-, trisubstituted alkenes
- formation of spirocyclic lactones
- aminogroup can be used for rearrangements

### General acid-mediated aminolactone formation using unactivated alkenes

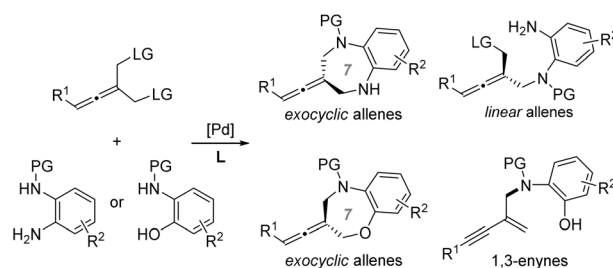
David Just, Carlos R. Gonçalves, Uroš Vezonik, Daniel Kaiser and Nuno Maulide\*



10812

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

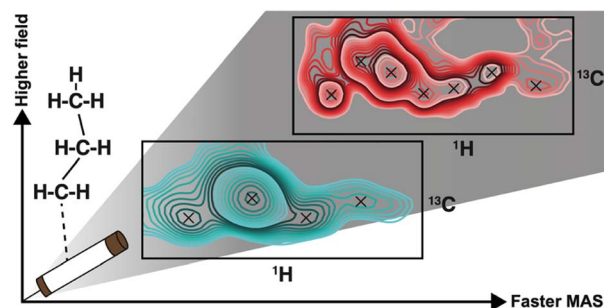
Pengfei Luo, Long Li, Xinfang Mao, Zheng Sun, Yingcheng Wang, Fangzhi Peng and Zhihui Shao\*



10824

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

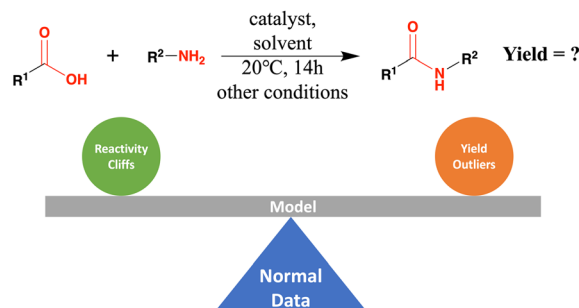
Morgane Callon,\* Dominique Luder, Alexander A. Malär, Thomas Wiegand, Václav Římal, Lauriane Lecoq, Anja Böckmann, Ago Samoson and Beat H. Meier\*



10835

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

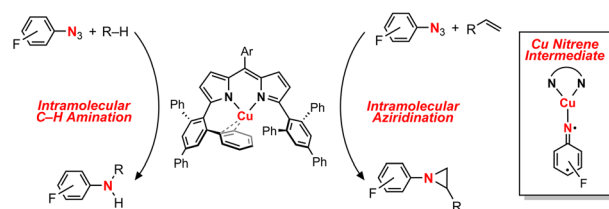
Zhen Liu, Yurii S. Moroz and Olexandr Isayev\*



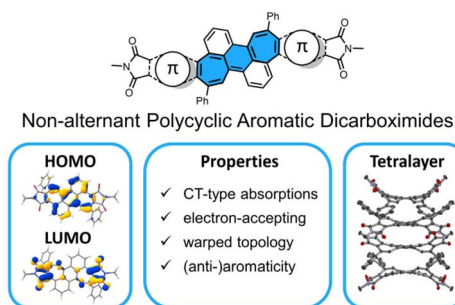
10847

### 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\*



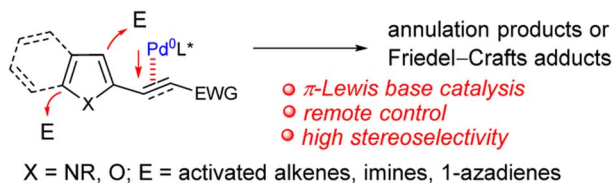
10861



### $\pi$ -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\*

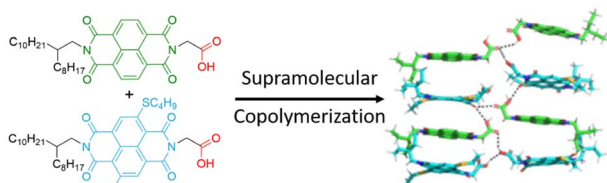
10867



### Asymmetric Friedel–Crafts reaction of unsaturated carbonyl-tethered heteroarenes via vinylogous activation of Pd<sup>0</sup>- $\pi$ -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\*

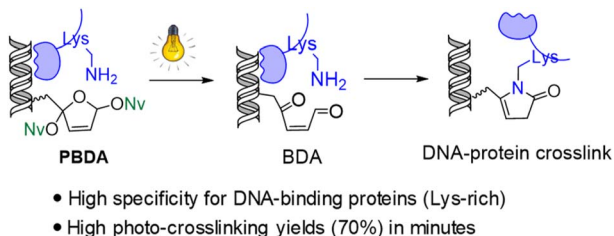
10875



### 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

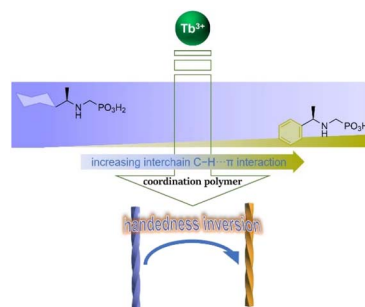
Jiahui Li, Zenghui Cui, Chaochao Fan, Yifei Zhou, Mengtian Ren and Chuangzheng Zhou\*



10892

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

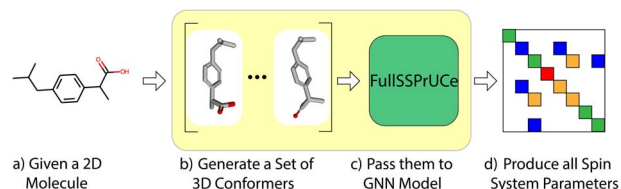
Chang-Yu Wang, Jia-Ge Jia, Guo-Guo Weng, Ming-Feng Qin, Kui Xu and Li-Min Zheng\*



10902

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

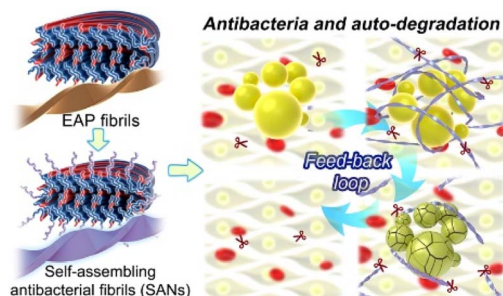
Jake Williams\* and Eric Jonas



10914

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

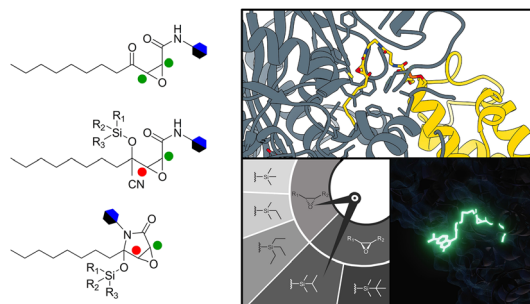
Fenghua Wang, Wencheng Xia, Mingming Zhang, Rongrong Wu, Xiaolu Song, Yun Hao, Yonghai Feng, Liwei Zhang, Dan Li, Wenyan Kang, Cong Liu\* and Lei Liu\*



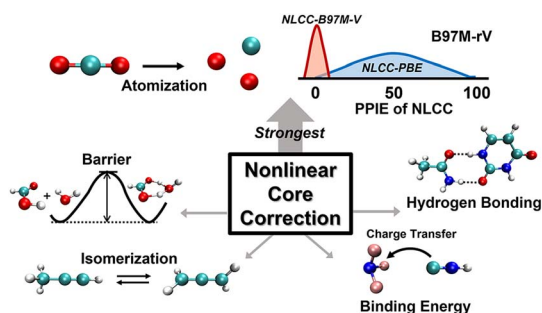
10925

### 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\*



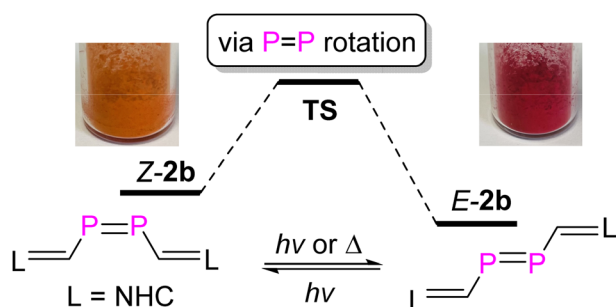
10934



### 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\*

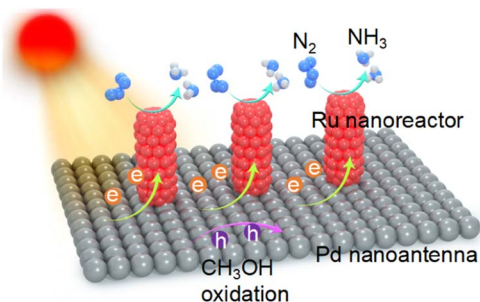
10944



### 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\*

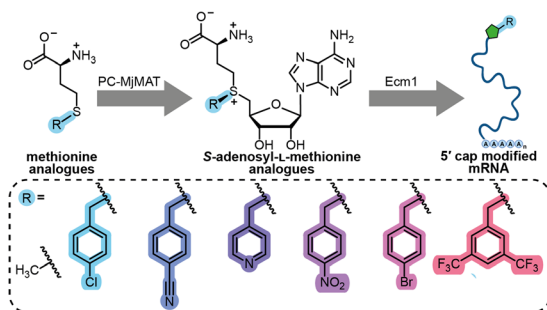
10953



### 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

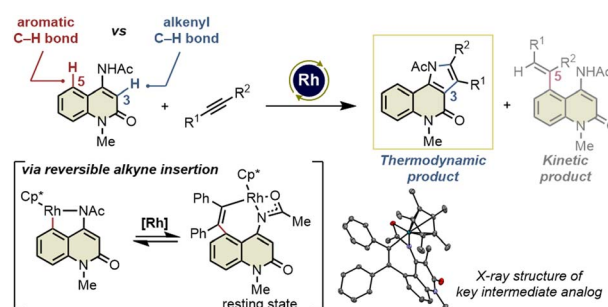
N. V. Cornelissen, R. Mineikaitė, M. Erguven, N. Muthmann, A. Peters, A. Bartels and A. Rentmeister\*



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\*

