

# Chemical Science

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## IN THIS ISSUE

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See Prince Ravat *et al.*,  
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Ehsan Faridi and Asim Swain  
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2024, 15, 11737.



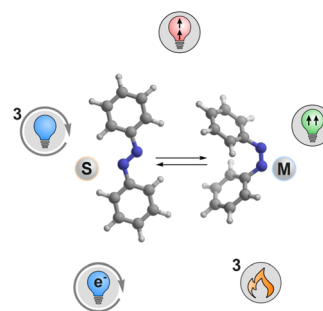
**Inside cover**  
See Rachel Codd *et al.*,  
pp. 11748–11760. Image  
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2024, 15, 11748.

## PERSPECTIVE

11684

### Detour to success: photoswitching *via* indirect excitation

Kim Kuntze, Jussi Isokuortti, Jacob J. van der Wal, Timo Laaksonen, Stefano Crespi,\* Nikita A. Durandin\* and Arri Priimagi\*

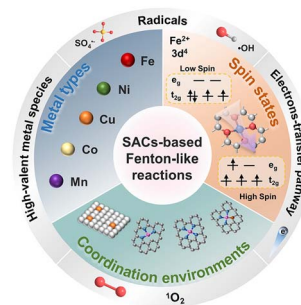


## REVIEWS

11699

### Correlating active sites and oxidative species in single-atom catalyzed Fenton-like reactions

Jie Miao, Yunyao Jiang, Xixi Wang, Xue Li, Yuan Zhu, Zongping Shao and Mingce Long\*



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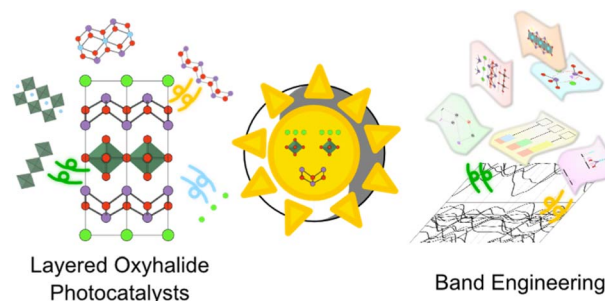
Fundamental questions  
Elemental answers

## REVIEWS

11719

**Band engineering of layered oxyhalide photocatalysts for visible-light water splitting**

Daichi Kato, Hajime Suzuki, Ryu Abe and Hiroshi Kageyama\*

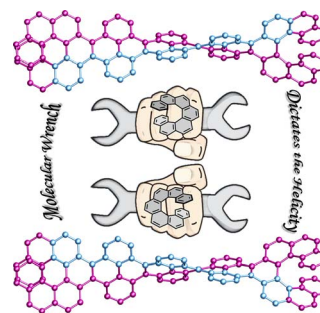


## EDGE ARTICLES

11737

**Helically twisted nanoribbons via stereospecific annulative  $\pi$ -extension reaction employing [7] helicene as a molecular wrench**

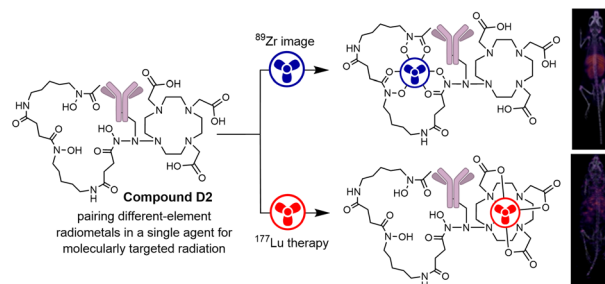
Asim Swain, Krzysztof Radacki, Holger Braunschweig and Prince Ravat\*



11748

**A first-in-class dual-chelator theranostic agent designed for use with imaging-therapy radiometal pairs of different elements**

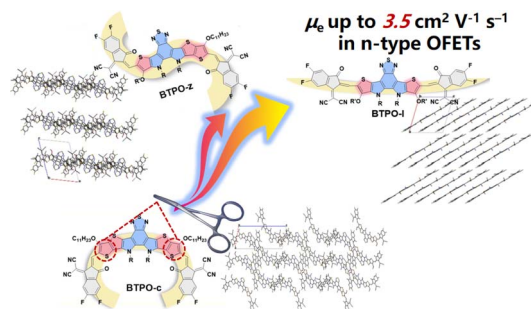
James L. Wood, Saikat Ghosh, Zachary H. Houston, Nicholas L. Fletcher, James Humphries, Karine Mardon, Dewan T. Akhter, William Tieu, Alesia Ivashkevich, Michael P. Wheatcroft, Kristofer J. Thurecht and Rachel Codd\*



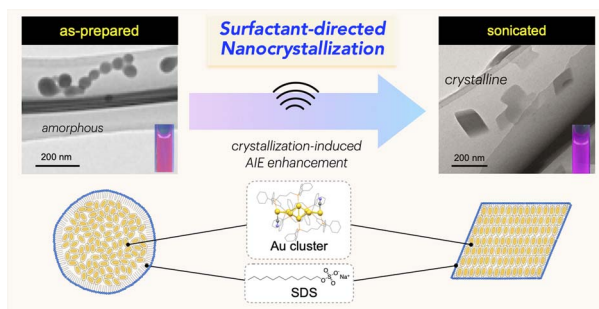
11761

**Molecular "backbone surgery" of electron-deficient heteroarenes based on dithienopyrrolobenzothiadiazole: conformation-dependent crystal structures and charge transport properties**

Yuzhong Chen, Zeng Wu, Zekun Chen, Shuixin Zhang, Wenhao Li, Yan Zhao, Yang Wang\* and Yunqi Liu



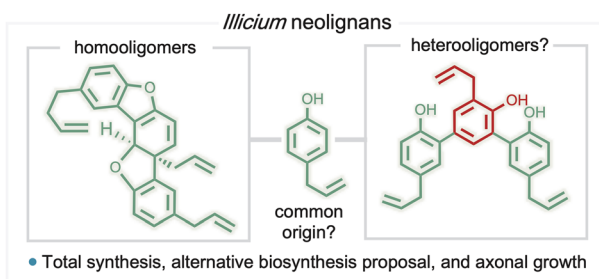
11775



### Controlled nanocrystallization of gold nanoclusters within surfactant envelopes: enhancing aggregation-induced emission in solution

Yuki Saito, Ayano Suda, Maki Sakai, Shogo Nakajima, Yukatsu Shichibu, Hayato Kanai, Yasuhiro Ishida\* and Katsuaki Konishi\*

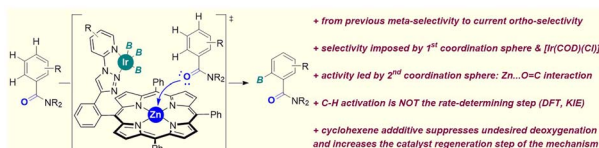
11783



### Total synthesis, biological evaluation and biosynthetic re-evaluation of *Illicium*-derived neolignans

Robert E. Arnold, Jan Saska, Raquel Mesquita-Ribeiro, Federico Dajas-Bailador, Laurence Taylor, William Lewis, Stephen Argent, Huiling Shao, Kendall N. Houk\* and Ross M. Denton\*

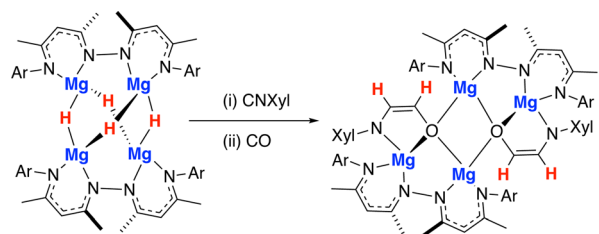
11794



### Repurposing a supramolecular iridium catalyst via secondary Zn...O=C weak interactions between the ligand and substrate leads to *ortho*-selective C(sp<sup>2</sup>)-H borylation of benzamides with unusual kinetics

Jonathan Trouvé, Vanessa Delahaye, Michele Tomasini, Purushothaman Rajeshwaran, Thierry Roisnel, Albert Poater\* and Rafael Gramage-Doria\*

11807



Selective Cross-Coupling - Templated by Cluster - New Ethene Amidolate

### Cross-coupling of CO and an isocyanide mediated by a tetrameric magnesium hydride cluster

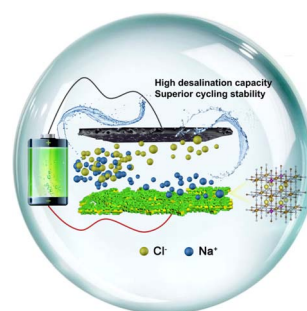
Wenbang Yang, Andrew J. P. White and Mark R. Crimmin\*



11814

## Enhanced redox kinetics of Prussian blue analogues for superior electrochemical deionization performance

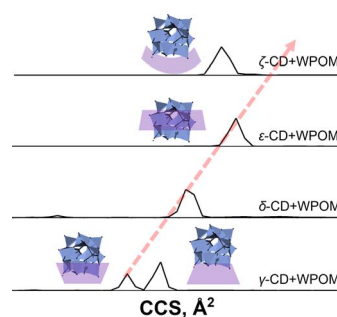
Jiabao Li, Ruoxing Wang, Lanlan Han, Tianyi Wang, Zeinhom M. El-Bahy, Yiyong Mai, Chengyin Wang,\* Yusuke Yamauchi\* and Xingtao Xu\*



11825

## The effect of host size on binding in host-guest complexes of cyclodextrins and polyoxometalates

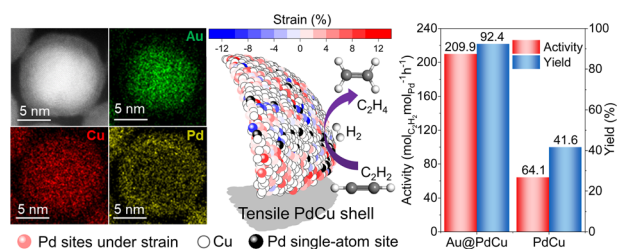
Pei Su,\* Xiao Zhu, Solita M. Wilson, Yuaning Feng, Hugo Y. Samayoa-Oviedo, Christian Sonnendecker, Andrew J. Smith, Wolfgang Zimmermann and Julia Laskin\*



11837

## Highly efficient semi-hydrogenation in strained ultrathin PdCu shell and the atomic deciphering for the unlocking of activity-selectivity

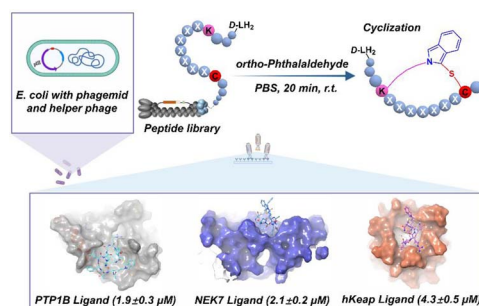
Fan Xue, Qiang Li,\* Weihua Ji, Mingxin Lv, Hankun Xu, Jianrong Zeng, Tianyi Li, Yang Ren, Lihui Zhou, Xin Chen, Jinxia Deng, Kun Lin and Xianran Xing\*



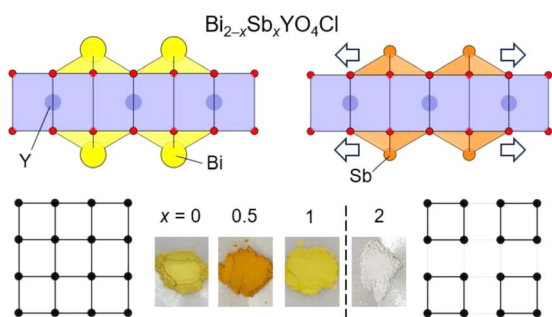
11847

## A facile strategy for the construction of a phage display cyclic peptide library for the selection of functional macrocycles

Hua Xiang, Liwen Bai, Xindan Zhang, Ting Dan, Peng Cheng, Xiaoqin Yang, Honglian Ai, Kai Li and Xinxiang Lei\*



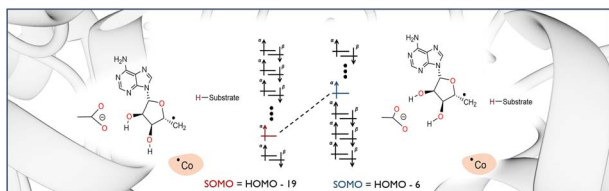
11856



### Internal strain-driven bond manipulation and band engineering in $\text{Bi}_{2-x}\text{Sb}_x\text{YO}_4\text{Cl}$ photocatalysts with triple fluorite layers

Artem Gabov, Daichi Kato,\* Hiroki Ubukata, Ryotaro Aso, Naoji Kakudou, Koji Fujita, Hajime Suzuki, Osamu Tomita, Akinori Saeki, Ryu Abe, Smagul Zh Karazhanov\* and Hiroshi Kageyama\*

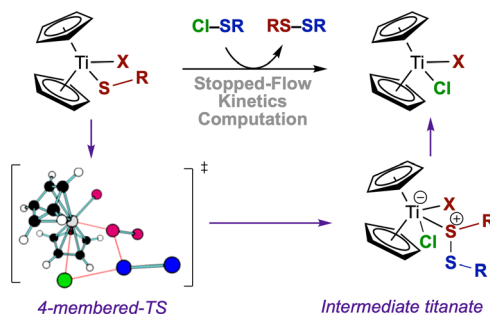
11865



### Non-Aufbau electronic structure in radical enzymes and control of the highly reactive intermediates

M. Hossein Khalilian and Gino A. DiLabio\*

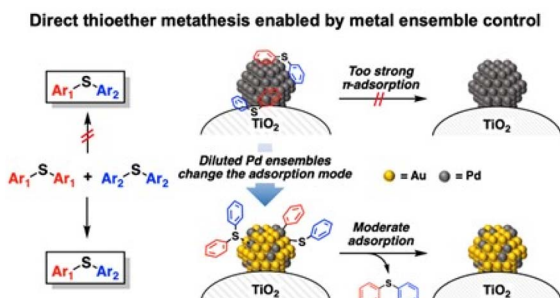
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### Kinetics of sulfur-transfer from titanocene (poly)sulfides to sulfenyl chlorides: rapid metal-assisted concerted substitution

Pedro H. Helou de Oliveira, Patrick J. Boaler, Guoxiong Hua, Nathan M. West, Robert T. Hembre, Jonathan M. Penney, Malik H. Al-Afyouni, J. Derek Woollins, Andrés García-Domínguez\* and Guy C. Lloyd-Jones\*

11884



### Heterogeneously catalyzed thioether metathesis by a supported Au-Pd alloy nanoparticle design based on Pd ensemble control

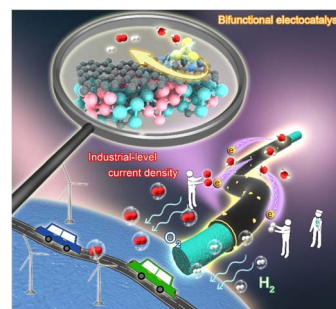
Takehiro Matsuyama, Takafumi Yatabe,\* Tomohiro Yabe and Kazuya Yamaguchi\*



11890

## Manipulating electron redistribution between iridium and Co<sub>6</sub>Mo<sub>6</sub>C bridging with a carbon layer leads to a significantly enhanced overall water splitting performance at industrial-level current density

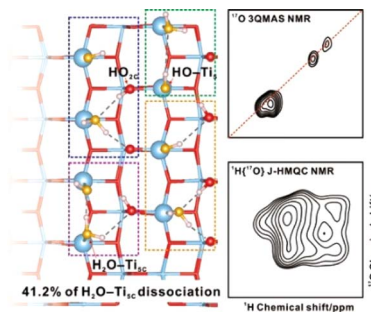
Weimo Li, Wenqiong Gou, Linfeng Zhang, Mengxiao Zhong, Siyu Ren, Guangtao Yu, Ce Wang, Wei Chen\* and Xiaofeng Lu\*



11902

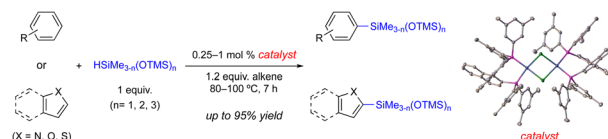
## Unraveling the atomic structure and dissociation of interfacial water on anatase TiO<sub>2</sub> (101) under ambient conditions with solid-state NMR spectroscopy

Longxiao Yang, Min Huang, Ningdong Feng,\* Meng Wang, Jun Xu, Ying Jiang, Ding Ma\* and Feng Deng\*



11912

## Intermolecular C–H silylations of arenes and heteroarenes with mono-, bis-, and tris(trimethylsiloxy)hydrosilanes: control of silane redistribution under operationally diverse approaches

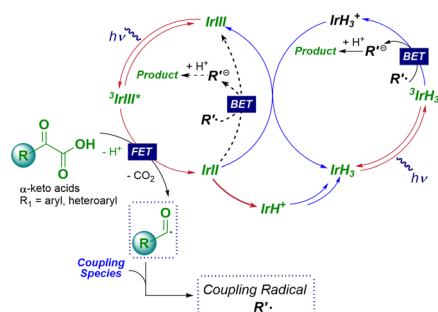


Noah Swann, Kiki Tang, Jihyeon Nam, Jooyeon Lee, Marek Domin, Thomas E. Shaw, Stosh A. Kozimor, Salina Som and Kangsang L. Lee\*

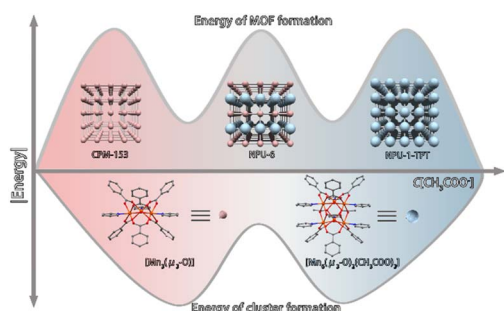
11919

## Multiphoton tandem photoredox catalysis of [Ir(dFCF<sub>3</sub>ppy)<sub>2</sub>(dtbbpy)]<sup>+</sup> facilitating radical acylation reactions

Zhicong Lin, Qian Zhou, Yan Liu, Chenli Chen, Jialong Jie\* and Hongmei Su



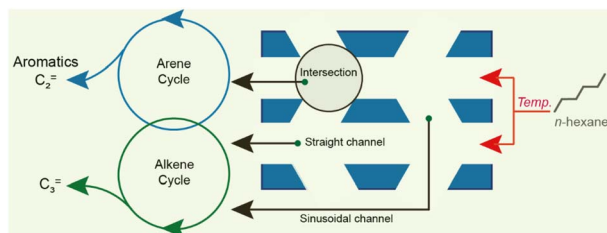
11928



### Ordered assembly of two different metal clusters with the same topological connectivity in one single coordination network

Jian-Wei Cao, Tao Zhang, Juan Chen, Jin-Bo Wang, Yu Wang and Kai-Jie Chen\*

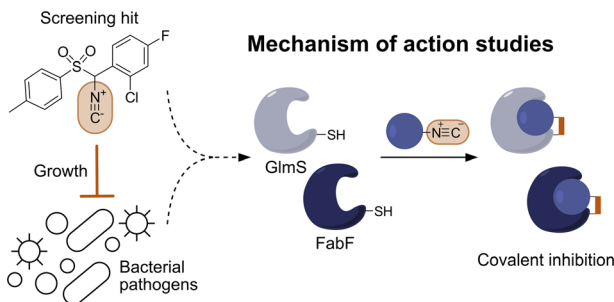
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### Selectivity descriptors of the catalytic *n*-hexane cracking process over 10-membered ring zeolites

Pandong Ma, Hexun Zhou, Yubing Li, Mengheng Wang, Stefan Adrian F. Nastase, Mengsi Zhu, Jiale Cui, Luigi Cavallo, Kang Cheng\* and Abhishek Dutta Chowdhury\*

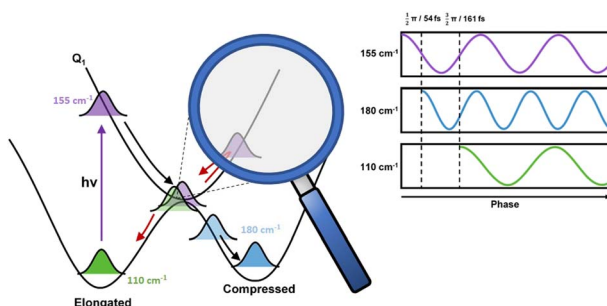
11946



### Isocyanides inhibit bacterial pathogens by covalent targeting of essential metabolic enzymes

Alexandra Geißler, Howard Junca, Andreas M. Kany, Lena J. Daumann, Anna K. H. Hirsch, Dietmar H. Pieper and Stephan A. Sieber\*

11956



### Tracking the conical intersection dynamics for the photoinduced Jahn–Teller switch of a Mn(III) complex

Ryan Phelps, Eleftheria Agapaki, Euan K. Brechin and J. Olof Johansson\*

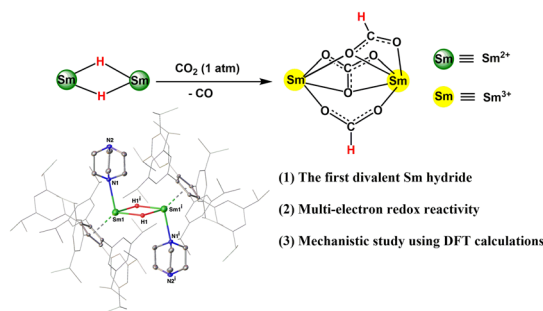




11965

### Multi-electron redox reactivity of a samarium(II) hydrido complex

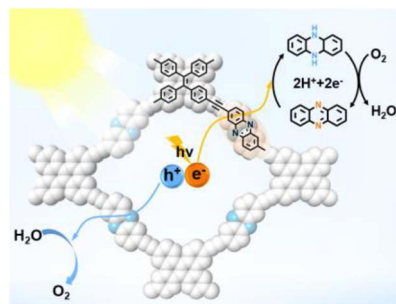
Xianghui Shi, Peng Deng, Thayalan Rajeshkumar, Laurent Maron\* and Jianhua Cheng\*



11972

### Leveraging phenazine and dihydrophenazine redox dynamics in conjugated microporous polymers for high-efficiency overall photosynthesis of hydrogen peroxide

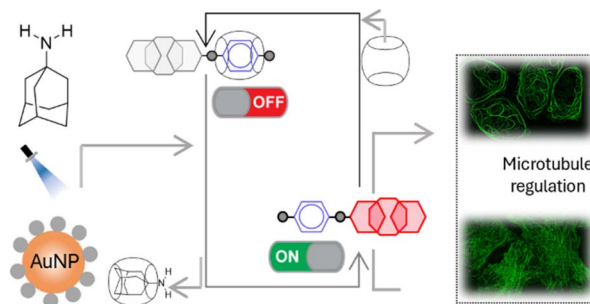
Shufan Feng, Lei Wang, Limei Tian, Ying Liu, Ke Hu, Hangxun Xu,\* Haifeng Wang\* and Jianli Hua\*



11981

### Regulation of microtubule dynamics and function in living cells via cucurbit[7]uril host-guest assembly

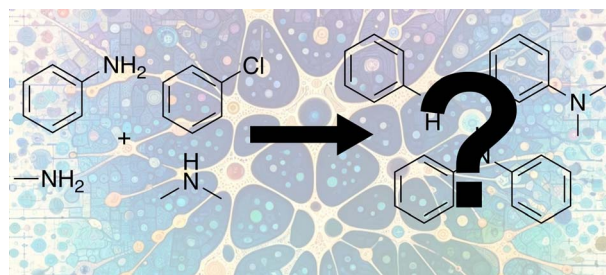
Akshay Saroha, Monica Swetha Bosco, Sneha Menon, Pratibha Kumari, Tanmoy Maity, Subinoy Rana, Sachin Kotak, Jagannath Mondal and Sarit S. Agasti\*



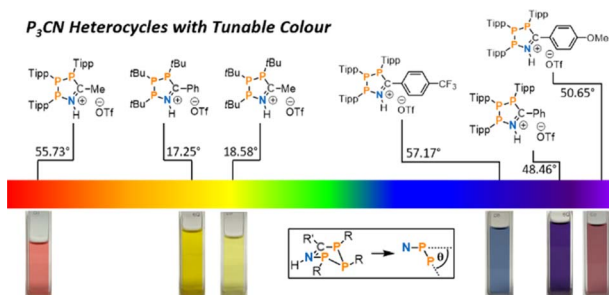
11995

### Deductive machine learning models for product identification

Tianfan Jin, Qiyuan Zhao, Andrew B. Schofield and Brett M. Savoie\*

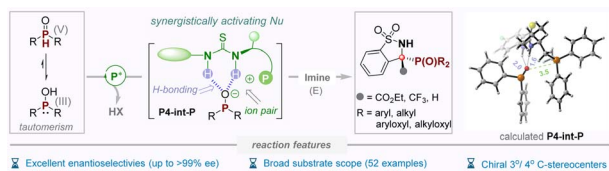


12006

***P*<sub>3</sub>CN Heterocycles with Tunable Colour****1,3-Dipolar cyclisation reactions of nitriles with sterically encumbered cyclic triphosphanes: synthesis and electronic structure of phosphorus-rich heterocycles with tunable colour**

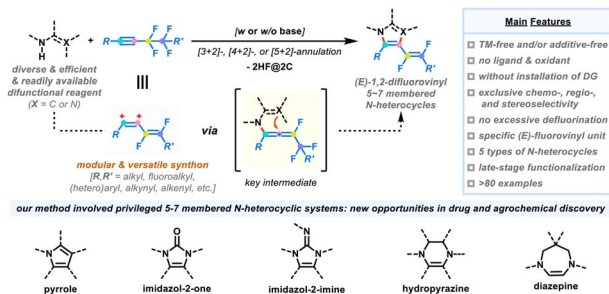
Mitchell A. Nascimento, Etienne A. LaPierre,\* Brian O. Patrick, Jade E. T. Watson, Lara Watanabe, Jeremy Rawson, Christian Hering-Junghans\* and Ian Manners

12017

**Synergistically activating nucleophile strategy enabled organocatalytic asymmetric P-addition of cyclic imines**

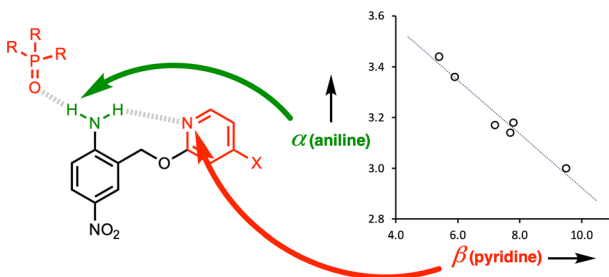
Hongkui Zhang, Jian-Ping Tan, Xiaoyu Ren, Fan Wang, Jia-Yan Zheng, Jiajia He, Yu Feng, Zhipeng Xu,\* Zhishan Su and Tianli Wang\*

12026

**Chemo-, regio-, and stereoselective tetrafunctionalization of fluoroalkynes enables divergent synthesis of 5-7-membered azacycles**

Jia-Wei Chen, Wen-Jun Ji, Xue-Ying Huang, Danhua Ge, Zhi-Liang Shen,\* Kai Guo\* and Xue-Qiang Chu\*

12036

**Negative cooperativity in the formation of H-bond networks involving primary anilines**

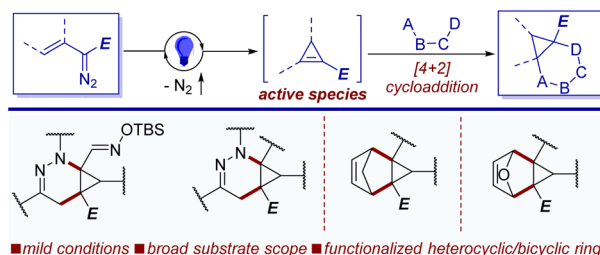
Fergal E. Hanna, Alexander J. Root, Markus Schade and Christopher A. Hunter\*



12042

### Photoinduced [4 + 2]-cycloaddition reactions of vinyl diazo compounds for the construction of heterocyclic and bicyclic rings

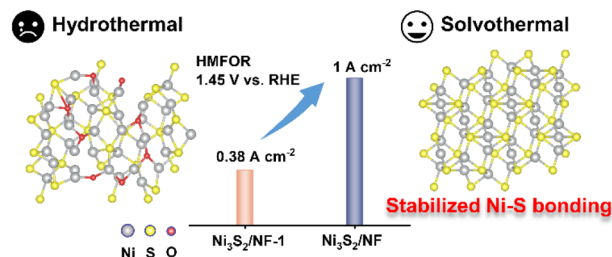
Ming Bao, Arnold R. Romero Bohórquez, Hadi Arman and Michael P. Doyle\*



12047

### Modulating Ni–S coordination in Ni<sub>3</sub>S<sub>2</sub> to promote electrocatalytic oxidation of 5-hydroxymethylfurfural at ampere-level current density

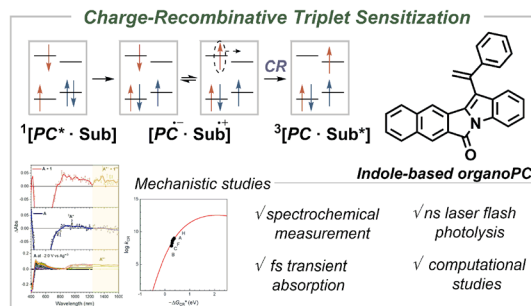
Lan Chen, Zhaohui Yang, Chuanyu Yan, Yijun Yin, Zhimin Xue,\* Yiting Yao, Shao Wang, Fanfei Sun\* and Tiancheng Mu\*



12058

### Charge-recombinative triplet sensitization of alkenes for DeMayo-type [2 + 2] cycloaddition

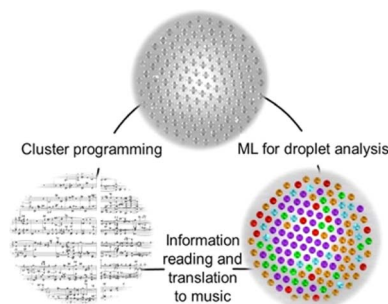
Yunjeong Lee, Byung Hak Jhun, Sihyun Woo, Seoyeon Kim, Jaehan Bae, Youngmin You\* and Eun Jin Cho\*



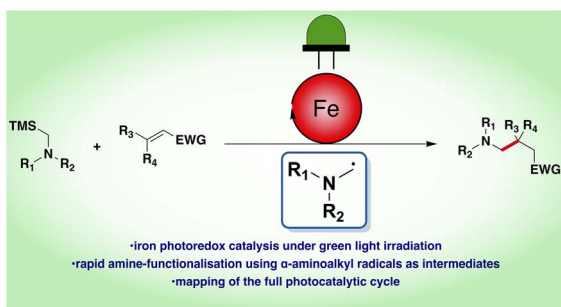
12067

### Observation of a chemical reaction in a levitating microdroplet cluster and droplet-generated music

Alexander A. Fedorets, Semyon Koltsov, Anton A. Muravev, Alexey Fotin, Pavel Zun, Nikita Orekhov, Michael Nosonovsky\* and Ekaterina V. Skorb\*



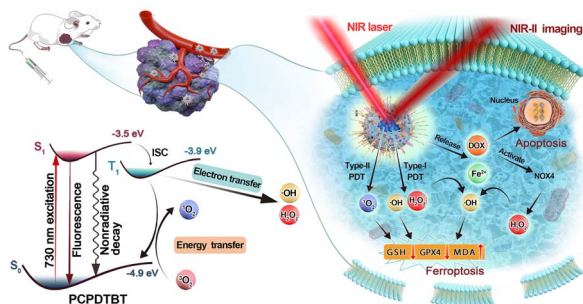
12077



### Aminomethylations of electron-deficient compounds—bringing iron photoredox catalysis into play

Aleksandra Ilic, Benjamin R. Strücker, Catherine E. Johnson, Simon Hainz, Reiner Lomoth\* and Kenneth Wärnmark\*

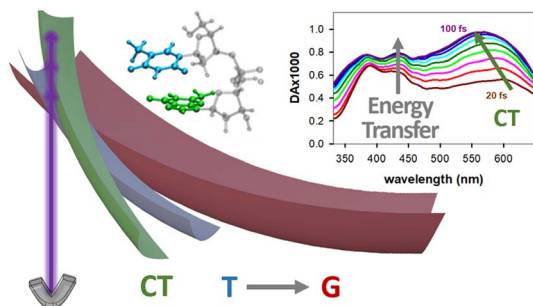
12086



### Confined semiconducting polymers with boosted NIR light-triggered H<sub>2</sub>O<sub>2</sub> production for hypoxia-tolerant persistent photodynamic therapy

Feng Lu, Lili Li, Meng Zhang, Chengwu Yu, Yonghui Pan, Fangfang Cheng, Wenbo Hu, Xiaomei Lu, Qi Wang\* and Quli Fan\*

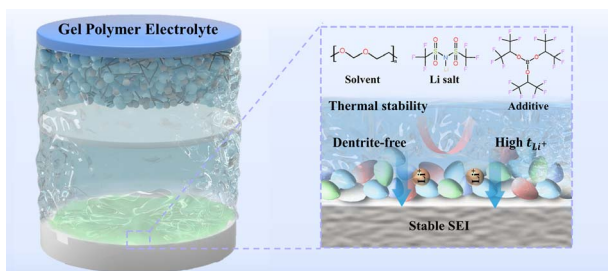
12098



### Real-time observation of sub-100-fs charge and energy transfer processes in DNA dinucleotides

Vasilis Petropoulos, Lara Martinez-Fernandez,\* Lorenzo Ubaldi, Margherita Maiuri, Giulio Cerullo,\* Evangelos Balanikas and Dimitra Markovitsi\*

12108



### *In situ* polymerization of 1,3-dioxolane and formation of fluorine/boron-rich interfaces enabled by film-forming additives for long-life lithium metal batteries

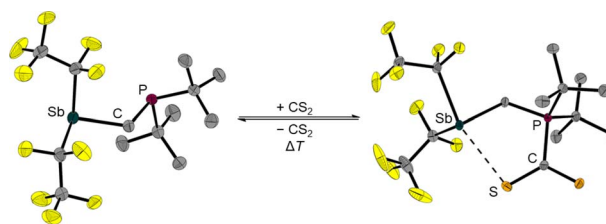
Ting Li, Kai Chen, Borui Yang, Kun Li, Bin Li, Miao He, Liu Yang, Anjun Hu\* and Jianping Long\*



12118

### A geminal antimony(III)/phosphorus(III) frustrated Lewis pair

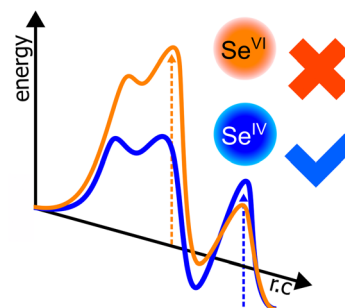
Jonas Krieff, Pia C. Trapp, Yury V. Vishnevskiy, Beate Neumann, Hans-Georg Stammler, Jan-Hendrik Lamm and Norbert W. Mitzel\*



12126

### Untangling the catalytic importance of the Se oxidation state in organoselenium-mediated oxygen-transfer reactions: the conversion of aniline to nitrobenzene

Andrea Madabeni, Damiano Tanini, Antonella Capperucci and Laura Orian\*



12138

### Flexible interactions of the rare-earth elements Y, La, and Lu with phosphorus in metallacyclohexane rings

Yury Minko, Taylor V. Fetrow, Shikha Sharma, Brenna K. Cashman and Aaron M. Tondreau\*

