

# Chemical Science

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## IN THIS ISSUE

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### Cover

See Hannah S. Shafaat et al., pp. 5916–5928. Image reproduced by permission of Luke C. Lewis from *Chem. Sci.*, 2024, 15, 5916.



### Inside cover

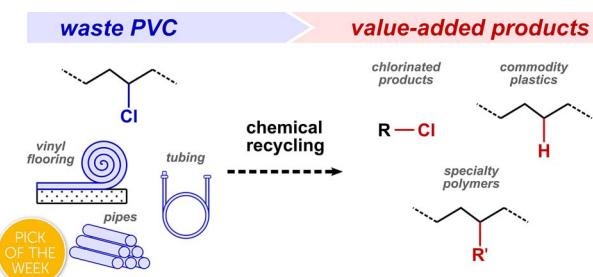
See Israel Fernández, Fernando Carrillo-Hermosilla, Joaquín García-Álvarez, David Elorriaga et al., pp. 5929–5937. Image reproduced by permission of Clara Becedóniz Plasencia from *Chem. Sci.*, 2024, 15, 5929.

## PERSPECTIVES

5802

### Revisiting poly(vinyl chloride) reactivity in the context of chemical recycling

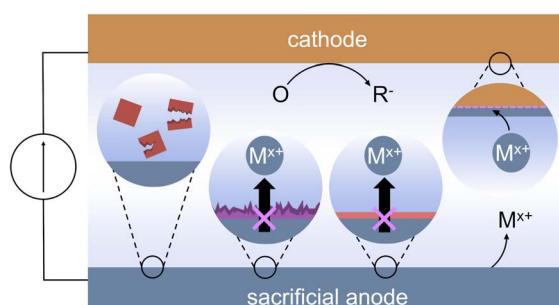
Rahul Kant Jha, Bertrand J. Neyhouse, Morgan S. Young, Danielle E. Fagnani and Anne J. McNeil\*



5814

### A guide to troubleshooting metal sacrificial anodes for organic electrosynthesis

Skyler D. Ware, Wendy Zhang, Weiyang Guan, Song Lin and Kimberly A. See\*



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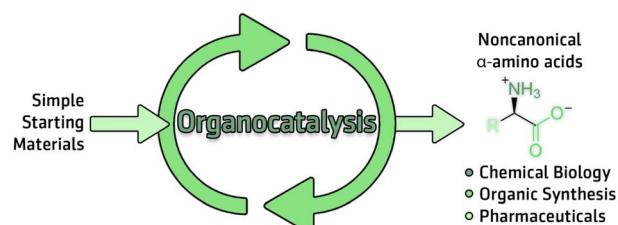


PERSPECTIVES

5832

## Enantioselective organocatalytic strategies to access noncanonical $\alpha$ -amino acids

Pietro Pecchini, Mariafrancesca Fochi,  
Francesca Bartoccini, Giovanni Piersanti\*  
and Luca Bernardi\*



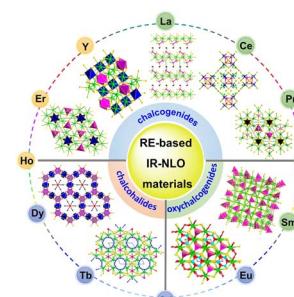
REVIEWS

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5869

# Rare-earth-based chalcogenides and their derivatives: an encouraging IR nonlinear optical material candidate

Ping Feng, Jia-Xiang Zhang, Mao-Yin Ran, Xin-Tao Wu,  
Hua Lin\* and Qi-Jiong Zhu\*

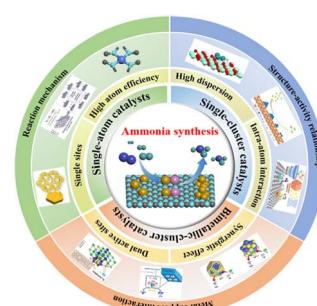


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5897

## Single-atom and cluster catalysts for thermocatalytic ammonia synthesis at mild conditions

Xuanbei Peng, Mingyuan Zhang, Tianhua Zhang,  
Yanliang Zhou\*, Jun Ni, Xiuyun Wang\*, and Lilong Jiang\*



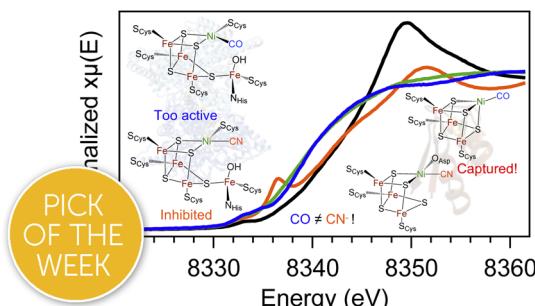
FDGF ARTICLES

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5916

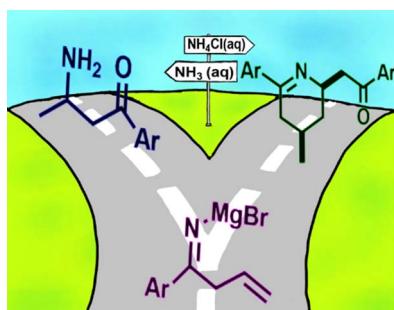
# Electronic isomerism in a heterometallic nickel–iron–sulfur cluster models substrate binding and cyanide inhibition of carbon monoxide dehydrogenase

Luke C. Lewis, José A. Sanabria-Gracia, Yuri Lee, Adam J. Jenkins and Hannah S. Shafaat\*



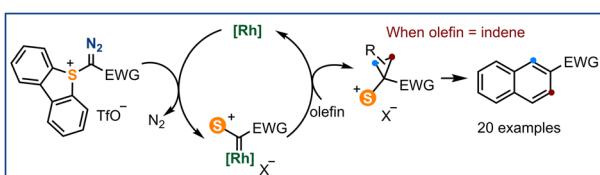
## EDGE ARTICLES

5929


**Addition of allyl Grignard to nitriles in air and at room temperature: experimental and computational mechanistic insights in pH-switchable synthesis**

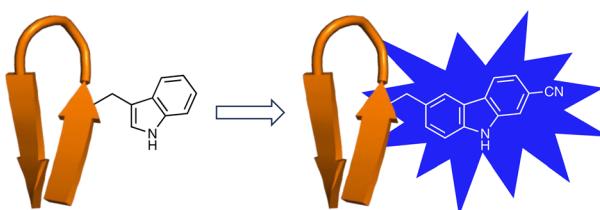
Blanca Parra-Cadenas, Israel Fernández,\* Fernando Carrillo-Hermosilla,\* Joaquín García-Álvarez\* and David Elorriaga\*

5938


**Reactivity of  $\alpha$ -diazo sulfonium salts: rhodium-catalysed ring expansion of indenes to naphthalenes**

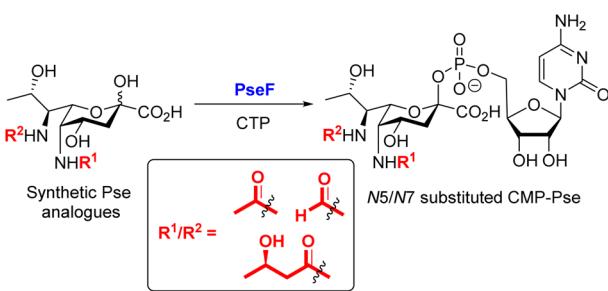
Sven Timmann, Tun-Hui Wu, Christopher Golz and Manuel Alcarazo\*

5944


**Fluorescent carbazole-derived  $\alpha$ -amino acids: structural mimics of tryptophan**

Rebecca Clarke, Liyao Zeng, Bethany C. Atkinson, Malcolm Kadodwala, Andrew R. Thomson\* and Andrew Sutherland\*

5950


**Investigation on the substrate specificity and  $N$ -substitution tolerance of PseF in catalytic transformation of pseudaminic acids to CMP-Pse derivatives**

Xing Guo, Yan Chu Cheung, Can Li, Han Liu,\* Pengfei Li,\* Sheng Chen\* and Xuechen Li\*

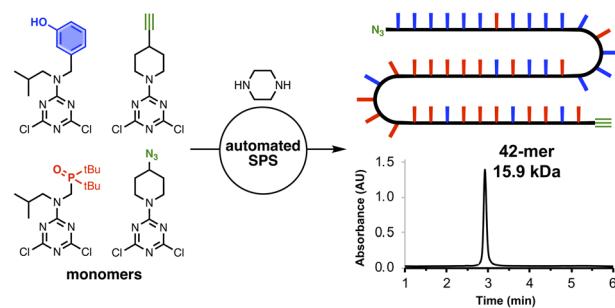


## EDGE ARTICLES

5957

**Efficient automated solid-phase synthesis of recognition-encoded melamine oligomers**

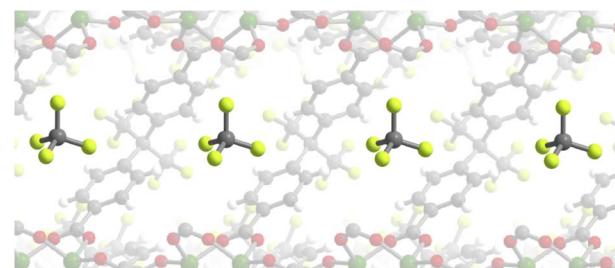
Mohit Dhiman, Rafel Cabot and Christopher A. Hunter\*



5964

**Selective adsorption of fluorinated super greenhouse gases within a metal–organic framework with dynamic corrugated ultramicropores**

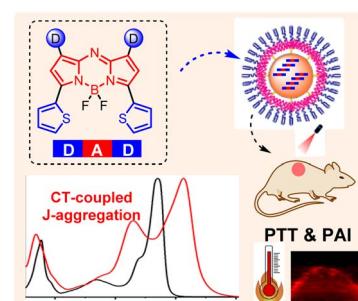
Bevan S. Whitehead, William W. Brennessel, Shane S. Michtavy, Hope A. Silva, Jaehwan Kim, Phillip J. Milner, Marc D. Porosoff and Brandon R. Barnett\*



5973

**Rational design of CT-coupled J-aggregation platform based on Aza-BODIPY for highly efficient phototherapy**

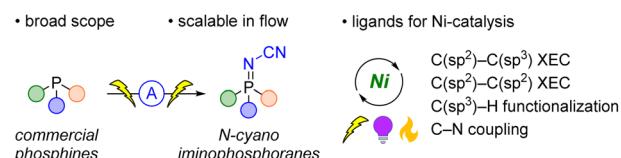
Shengmei Wu, Wenze Zhang, Chaoran Li, Zhigang Ni, Weifeng Chen, Lizhi Gai,\* Jiangwei Tian,\* Zijian Guo and Hua Lu\*



5980

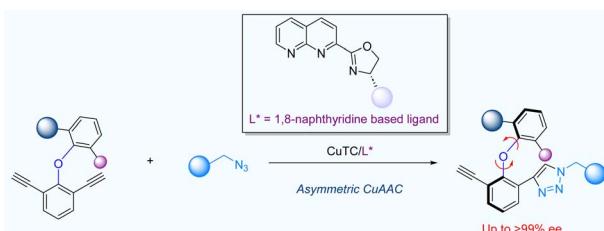
**Electrosynthesis of iminophosphoranes and applications in nickel catalysis**

Velabo Mdluli, Dan Lehnher,\* Yu-hong Lam,\* Mohammad T. Chaudhry, Justin A. Newman, Jimmy O. DaSilva and Erik L. Regalado



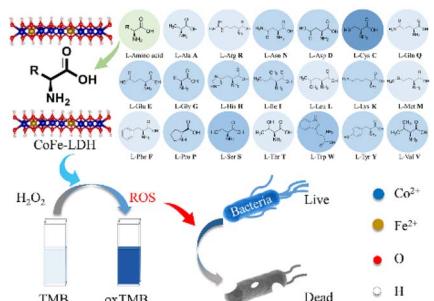
## EDGE ARTICLES

5993


**Copper-catalyzed atroposelective synthesis of C–O axially chiral compounds enabled by chiral 1,8-naphthyridine based ligands**

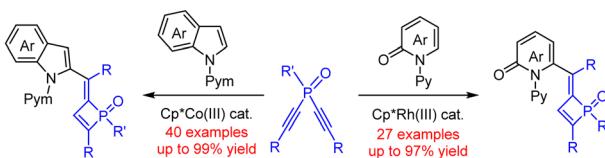
Lei Dai, Xueling Zhou, Jiami Guo, Qingqin Huang and Yixin Lu\*

6002


**Facile preparation of high-efficiency peroxidase mimics: modulation of the catalytic microenvironment of LDH nanozymes through defect engineering induced by amino acid intercalation**

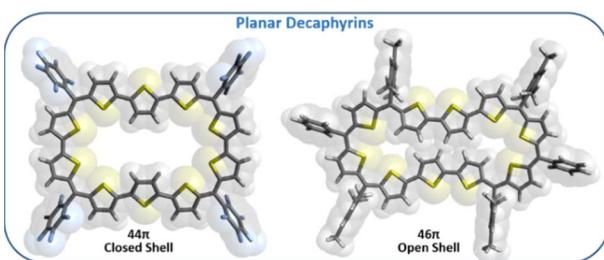
Dong Han, Kui Yang, Lanlan Chen, Zhaosheng Zhang, Chen Wang, Hongyuan Yan\* and Jia Wen\*

6012


**Cobalt- or rhodium-catalyzed synthesis of 1,2-dihydrophosphate oxides via C–H activation and formal phosphoryl migration**

Shengbo Xu, Ruijie Mi, Guangfan Zheng\* and Xingwei Li\*

6022


**Open shell  $(4n + 2)\pi$  and closed shell  $4n\pi$  planar core-modified decaphyrins**

Pragati Shukla, Madan D. Ambhare and Venkataramanarao G. Anand\*

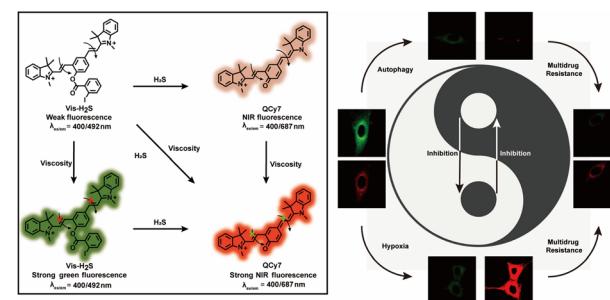


## EDGE ARTICLES

6028

**Near-infrared imaging for visualizing the synergistic relationship between autophagy and NFS1 protein during multidrug resistance using an ICT–TICT integrated platform**

Wei Hu, Yifan He, Haixian Ren,\* Li Chai, Haiyan Li, Jianbin Chen, Chunya Li,\* Yanying Wang\* and Tony D. James\*



6036

**Combining geometric constraint and redox non-innocence within an ambiphilic PBP pincer ligand**

Peter Coburger, Ana Guilherme Buzanich, Franziska Emmerling and Josh Abbenseth\*

**Transition Metal Complexes of a Redox Active PBP Pincer Ligand**

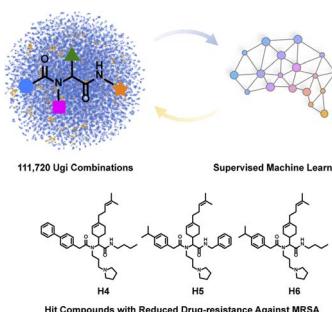
- Combination of Geometric Constraint and a Redox Active Support
- Ambiphilic Bi-M bonding in Coordination Compounds
- Bonding Analysis via XANES, XRD, UV/vis and (TD)-DFT



6044

**Combinatorial discovery of antibacterials via a feature-fusion based machine learning workflow**

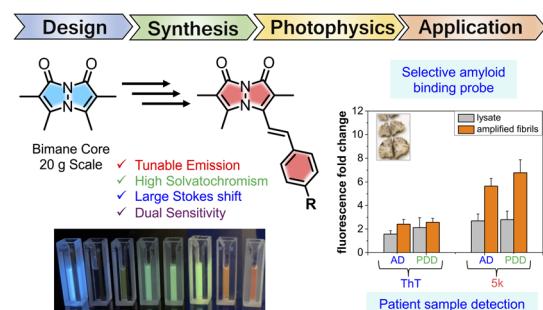
Cong Wang, Yuhui Wu, Yunfan Xue, Lingyun Zou, Yue Huang, Peng Zhang\* and Jian Ji\*



6053

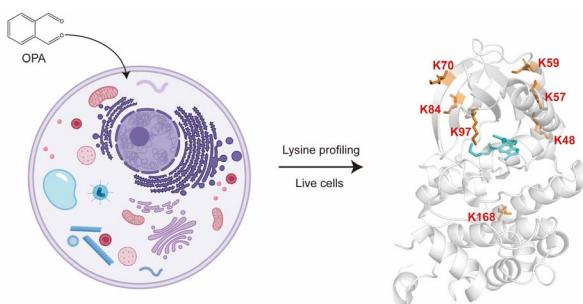
**Highly tunable bimane-based fluorescent probes: design, synthesis, and application as a selective amyloid binding dye**

Yarra Venkatesh, Nicholas P. Marotta, Virginia M.-Y. Lee and E. James Petersson\*



## EDGE ARTICLES

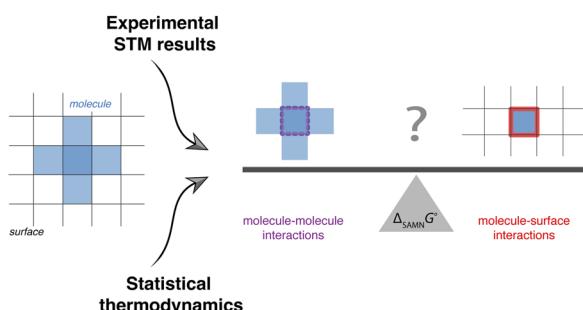
6064



**Protein painting for structural and binding site analysis via intracellular lysine reactivity profiling with *o*-phthalaldehyde**

Zhenxiang Zheng, Ya Zeng, Kunjia Lai, Bin Liao, Pengfei Li and Chris Soon Heng Tan\*

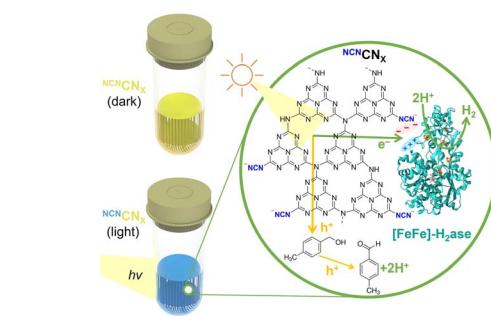
6076



**On the origin of cooperativity effects in the formation of self-assembled molecular networks at the liquid/solid interface**

Tamara Rinkovec, Demian Kalebic, Wim Dehaen, Stephen Whitelam, Jeremy N. Harvey\* and Steven De Feyter\*

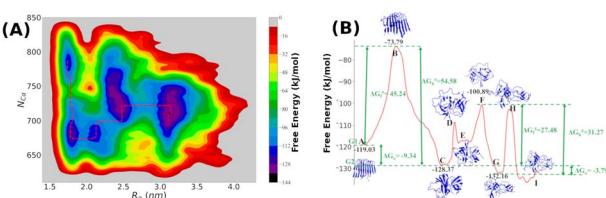
6088



**Electrostatic [FeFe]-hydrogenase–carbon nitride assemblies for efficient solar hydrogen production**

Yongpeng Liu, Carolina Pulignani, Sophie Webb, Samuel J. Cobb, Santiago Rodríguez-Jiménez, Dongseok Kim, Ross D. Milton and Erwin Reisner\*

6095



**Can local heating and molecular crowders disintegrate amyloid aggregates?**

Naresh Kumar, Prabir Khatua and Sudipta Kumar Sinha

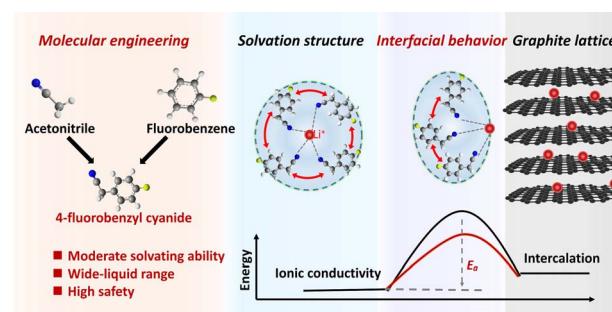


## EDGE ARTICLES

6106

**4-Fluorobenzyl cyanide, a sterically-hindered solvent expediting interfacial kinetics in lithium-ion batteries**

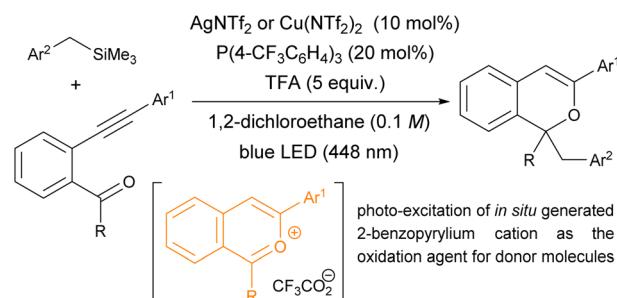
Mingsheng Qin, Ziqi Zeng,\* Qiang Wu, Xiaowei Liu, Qijun Liu, Shijie Cheng and Jia Xie\*



6115

**Consecutive  $\pi$ -Lewis acidic metal-catalysed cyclisation/photochemical radical addition promoted by *in situ* generated 2-benzopyrylium as the photoredox catalyst**

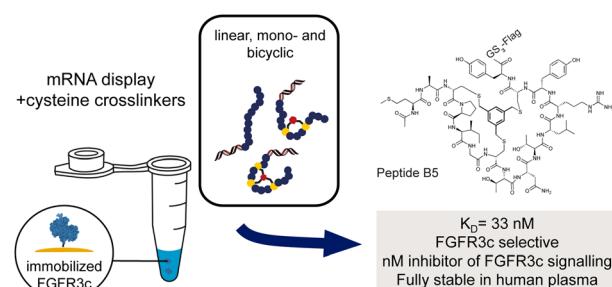
Masahiro Terada,\* Ryohei Yazaki, Ren Obayashi, Zen Iwasaki, Shigenobu Umemiya and Jun Kikuchi



6122

**An efficient mRNA display protocol yields potent bicyclic peptide inhibitors for FGFR3c: outperforming linear and monocyclic formats in affinity and stability**

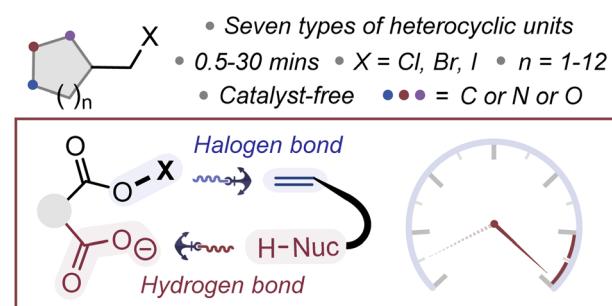
Camille Villequey,\* Silvana S. Zurmühl, Christian N. Cramer, Bhaskar Bhushan, Birgitte Andersen, Qianshen Ren, Haimo Liu, Xinping Qu, Yang Yang, Jia Pan, Qiuju Chen and Martin Münzel



6130

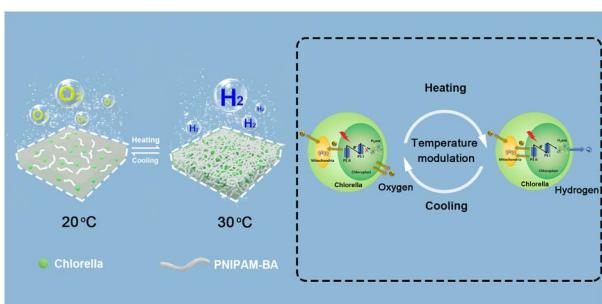
**Intramolecular chaperone-assisted dual-anchoring activation (ICDA): a suitable preorganization for electrophilic halocyclization**

Xihui Yang, Haowei Gao, Jiale Yan, Jia Zhou\* and Lei Shi\*



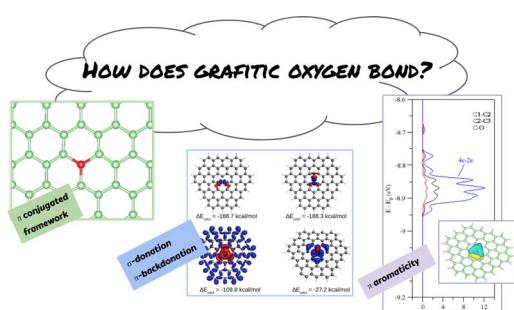
## EDGE ARTICLES

6141


**Temperature modulated sustainable on/off photosynthesis switching of microalgae towards hydrogen evolution**

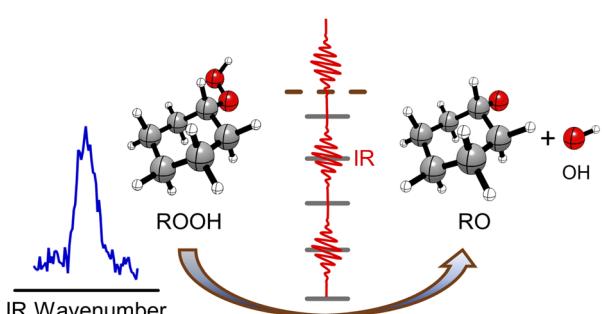
Shangsong Li, Zhijun Xu, Song Lin, Luxuan Li, Yan Huang, Xin Qiao and Xin Huang\*

6151


**Deciphering the chemical bonding of the trivalent oxygen atom in oxygen doped graphene**

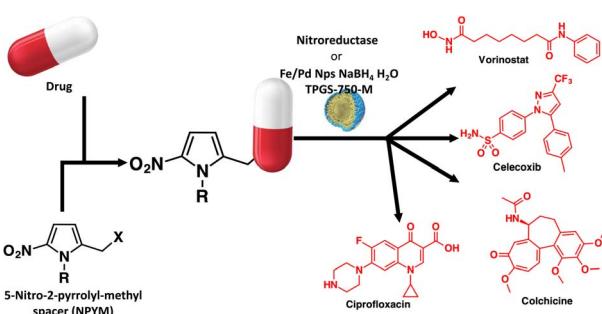
Andoni Ugartemendia, Irene Casademont-Reig, Lili Zhao, Zuxian Zhang, Gernot Frenking, Jesus M. Ugalde, Aran Garcia-Lekue\* and Elisa Jimenez-Izal\*

6160


**Vibrational spectroscopy and dissociation dynamics of cyclohexyl hydroperoxide**

Tarun Kumar Roy, Yujie Qian, Elizabeth Karlsson, Rawan Rabayah, Christopher A. Sojda, Marisa C. Kozlowski, Tolga N. V. Karsili and Marsha I. Lester\*

6168


**A novel bioresponsive self-immolative spacer based on aza-quinone methide reactivity for the controlled release of thiols, phenols, amines, sulfonamides or amides**

Elena Ermini, Annalaura Brai, Elena Cini, Federica Finetti, Giuseppe Giannini, Daniele Padula, Lucrezia Paradisi, Federica Poggialini, Lorenza Trabalzini, Paola Tolu and Maurizio Taddei\*



## EDGE ARTICLES

6178

**Visible-light-driven alkene dicarboxylation with formate and CO<sub>2</sub> under mild conditions**

Fulin Zhang, Xiao-Yang Wu, Pan-Pan Gao, Hao Zhang, Zhu Li, Shangde Ai and Gang Li\*

