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# Chemical Science

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## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 14(44) 12389–12800 (2023)

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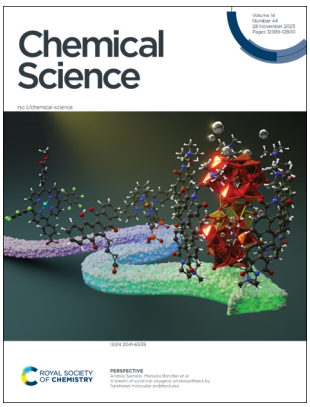


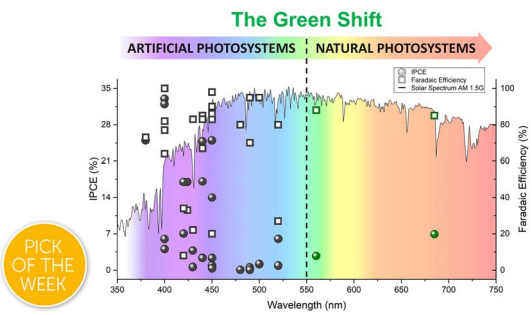

**Inside cover**
See Andrea Sartorel, Marcella Bonchio *et al.*, pp. 12402–12429. Image reproduced by permission of Marcella Bonchio from *Chem. Sci.*, 2023, **14**, 12402. Robin N. Dürr is thankfully acknowledged for designing and creating the cover artwork.

## PERSPECTIVES

12402

**A breath of sunshine: oxygenic photosynthesis by functional molecular architectures**

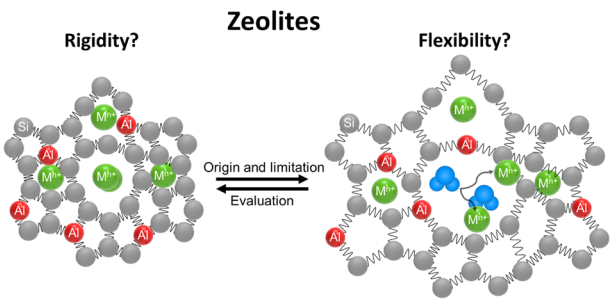
Thomas Gobbato, Giulia Alice Volpato, Andrea Sartorel* and Marcella Bonchio*




12430

**Flexibility in zeolites: origin, limits, and evaluation**

Sajjad Ghojavand, Eddy Dib and Svetlana Mintova*



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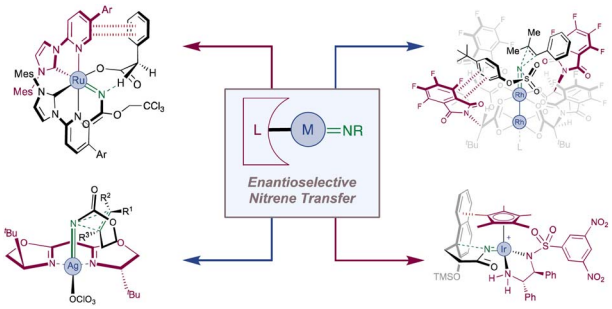
## REVIEW

12447

**Catalytic, asymmetric carbon–nitrogen bond formation using metal nitrenoids: from metal–ligand complexes *via* metalloporphyrins to enzymes**

Alexander Fanourakis and Robert J. Phipps*

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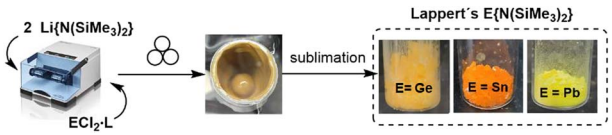
12477

**Fast and scalable solvent-free access to Lappert's heavier tetrylenes $E\{N(SiMe_3)_2\}_2$ (E = Ge, Sn, Pb) and $ECl\{N(SiMe_3)_2\}$ (E = Ge, Sn)**

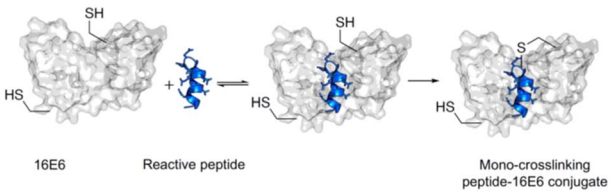
Javier A. Cabeza, Javier F. Reynes, Felipe García,* Pablo García-Álvarez* and Rubén García-Soriano




12484

**Discovery of reactive peptide inhibitors of human papillomavirus oncoprotein E6**

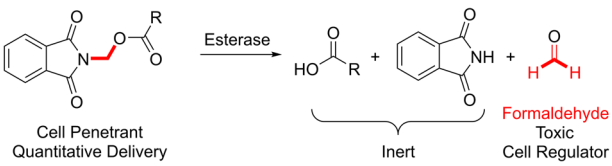
Xiyun Ye, Peiyuan Zhang, Jason Tao, John C. K. Wang, Amirhossein Mafi, Nathalie M. Grob, Anthony J. Quartararo, Hannah T. Baddock, Leanne J. G. Chan, Fiona E. McAllister, Ian Foe, Andrei Loas, Dan L. Eaton, Qi Hao, Aaron H. Nile* and Bradley L. Pentelute*




12498

***N*-Acyloxymethyl-phthalimides deliver genotoxic formaldehyde to human cells**

Vicki L. Emms, Liam A. Lewis, Lilla Beja, Natasha F. A. Bulman, Elisabete Pires, Frederick W. Muskett, James S. O. McCullagh, Lonnie. P. Swift,* Peter J. McHugh* and Richard J. Hopkinson*



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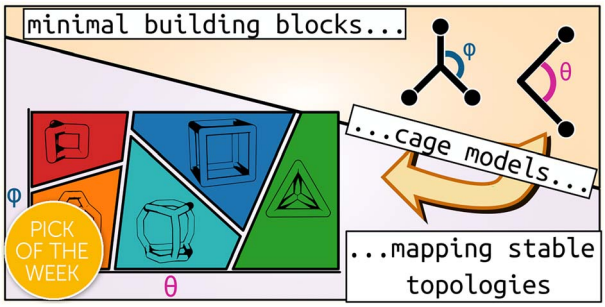
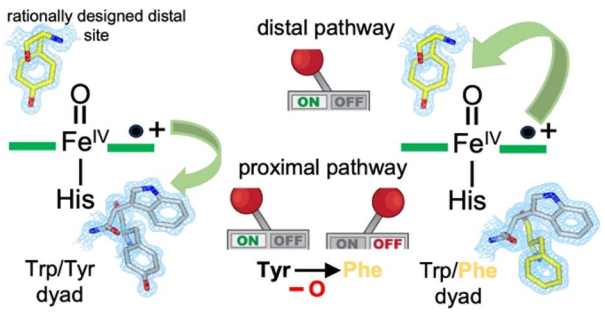



### Systematic exploration of accessible topologies of cage molecules *via* minimalistic models

Andrew Tarzia,* Emma H. Wolpert, Kim E. Jelfs and Giovanni M. Pavan*

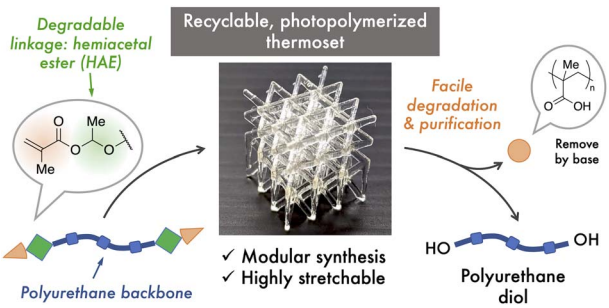
12518




### New insights into controlling radical migration pathways in heme enzymes gained from the study of a dye-decolorising peroxidase

Marina Lučić, Michael T. Wilson, Jacob Pullin, Michael A. Hough, Dimitri A. Svistunenko* and Jonathan A. R. Worrall*

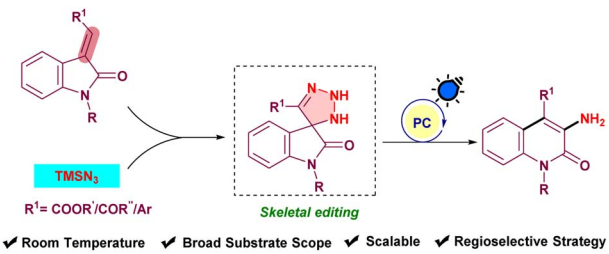
12535




### Stretchable, recyclable thermosets *via* photopolymerization and 3D printing of hemiacetal ester-based resins

You-Chi Mason Wu, Gloria Chyr, Hyunchang Park, Anna Makar-Limanov, Yuran Shi, Joseph M. DeSimone and Zhenan Bao*

12541




### Skeletal rearrangement through photocatalytic denitrogenation: access to C-3 aminoquinolin-2(1*H*)-ones

Swati Singh, Gopal Chakrabortty and Sudipta Raha Roy*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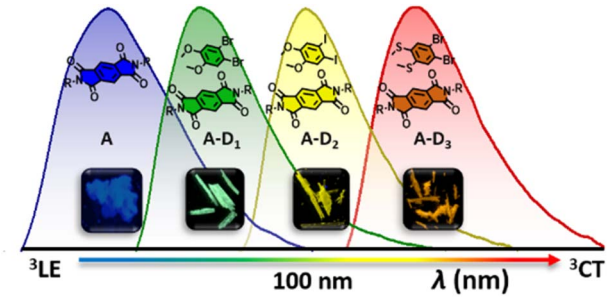
## EDGE ARTICLES

12548

**Revisiting organic charge-transfer cocrystals for wide-range tunable, ambient phosphorescence**

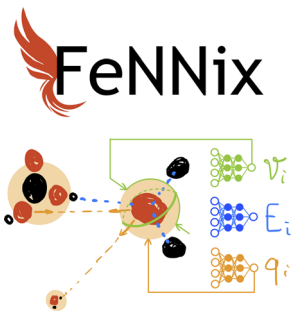
Anju Ajayan Kongasseri, Shagufi Naz Ansari, Swadhin Garain, Sopan M. Wagalgave and Subi J. George*




12554

**Force-field-enhanced neural network interactions: from local equivariant embedding to atom-in-molecule properties and long-range effects**

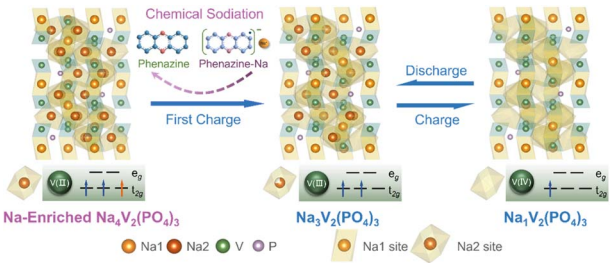
Thomas Plé,* Louis Lagardère* and Jean-Philip Piquemal*




12570

**Controllable synthesis of a Na-enriched $Na_4V_2(PO_4)_3$ cathode for high-energy sodium-ion batteries: a redox-potential-matched chemical sodiation approach**

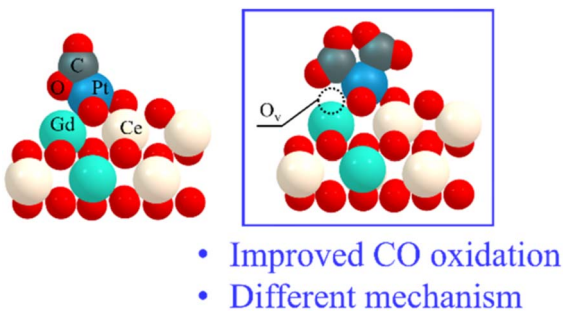
Mingli Xu, Fengxue Zhang, Yanhui Zhang, Chen Wu, Xue Zhou, Xinping Ai and Jiangfeng Qian*




12582

**Active sites of atomically dispersed Pt supported on Gd-doped ceria with improved low temperature performance for CO oxidation**

Yuanyuan Li,* Haodong Wang, Haohong Song, Ning Rui, Matthew Kottwitz, Sanjaya D. Senanayake, Ralph G. Nuzzo, Zili Wu, De-en Jiang and Anatoly I. Frenkel*



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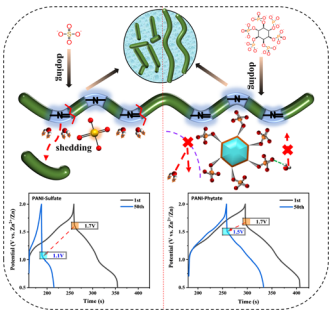
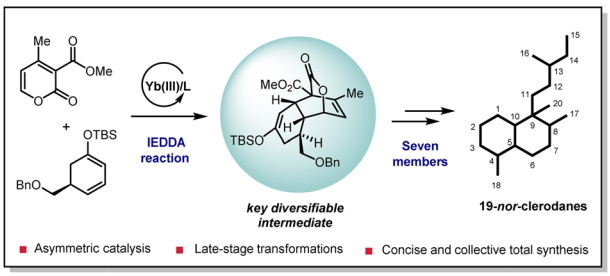



### Enhancing organic cathodes of aqueous zinc-ion batteries *via* utilizing steric hindrance and electron cloud equalization

Guanzhong Ma, Zhengyu Ju, Xin Xu, Yunfei Xu, Yao Sun, Yaqun Wang,* Guoxin Zhang, Mian Cai, Lijia Pan* and Guihua Yu*

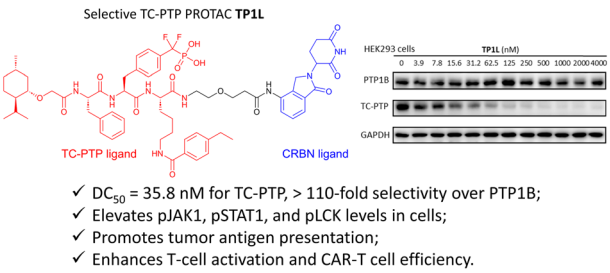
12598




### Enantioselective and collective total synthesis of pentacyclic 19-*nor*-clerodanes

Zhi-Mao Zhang, Junliang Zhang and Quan Cai*

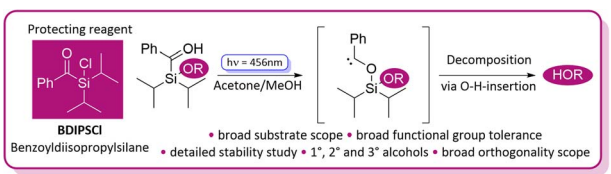
12606




### Discovery of a selective TC-PTP degrader for cancer immunotherapy

Jinmin Miao, Jiajun Dong, Yiming Miao, Yunpeng Bai, Zihan Qu, Brenson A. Jassim, Bo Huang, Quyen Nguyen, Yuan Ma, Allison A. Murray, Jinyue Li, Philip S. Low and Zhong-Yin Zhang*

12615




### Benzoyldiisopropylchlorosilane: a visible light photocleavable alcohol protecting group

Florian Lind, Kirill Markelov and Armido Studer*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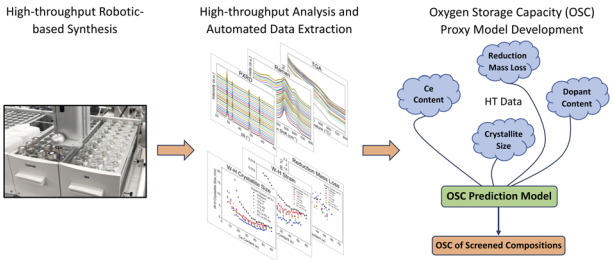
## EDGE ARTICLES

12621

**A proxy for oxygen storage capacity from high-throughput screening and automated data analysis**

Jack J. Quayle, Alexandros P. Katsoulidis, John B. Claridge, Andrew P. E. York, David Thompsett and Matthew J. Rosseinsky*

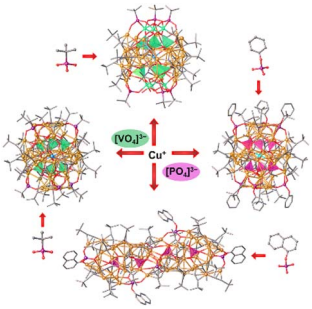



Accelerated discovery of high OSC Materials through high-throughput synthesis, analysis, and proxy models.

12637

**Template-assisted synthesis of isomeric copper(I) clusters with tunable structures showing photophysical and electrochemical properties**

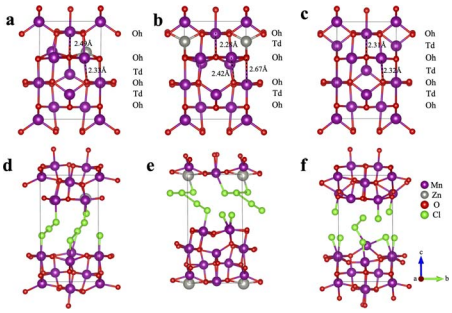
Jun-Jie Fang, Zheng Liu, Yang-Lin Shen, Yun-Peng Xie* and Xing Lu*




12645

**Reversible Cl/Cl⁻ redox in a spinel $Mn_3O_4$ electrode**

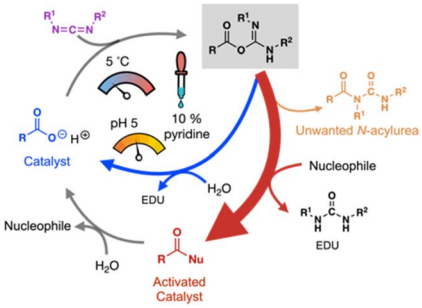
Sean K. Sandstrom, Qiuyao Li, Yiming Sui, Mason Lyons, Chun-Wai Chang, Rui Zhang, Heng Jiang, Mingliang Yu, David Hoang, William F. Stickle, Huolin L. Xin,* Zhenxing Feng,* De-en Jiang* and Xiulei Ji*




12653

**Suppressing catalyst poisoning in the carbodiimide-fueled reaction cycle**

Xiaoyao Chen, Héctor Soria-Carrera, Oleksii Zozulia and Job Boekhoven*



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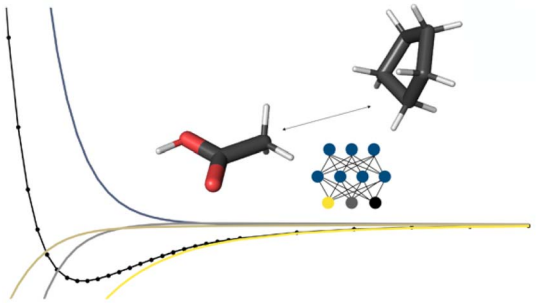
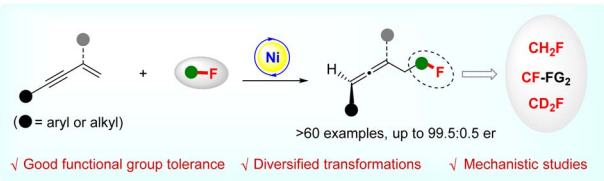
12661



**Hybrid classical/machine-learning force fields for the accurate description of molecular condensed-phase systems**

Moritz Thürlemann and Sereina Riniker*

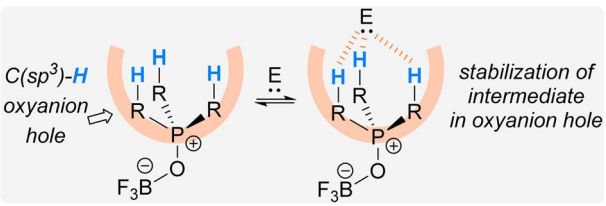
12676




**Nickel-catalysed asymmetric hydromonofluoromethylation of 1,3-enynes for enantioselective construction of monofluoromethyl-tethered chiral allenes**

Ying Zhang, Jimin Yang, Yu-Long Ruan, Ling Liao, Chuang Ma, Xiao-Song Xue* and Jin-Sheng Yu*

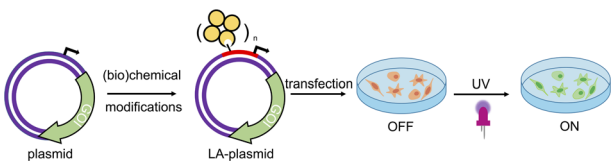
12684




**Trialkylphosphonium oxoborates as C(sp$^3$)–H oxyanion holes and their application in catalytic chemoselective acetalization**

Vincent Ming-Yau Leung, Hong-Chai Fabio Wong, Chun-Man Pook, Ying-Lung Steve Tse* and Ying-Yeung Yeung*

12693




**Sequence-independent, site-specific incorporation of chemical modifications to generate light-activated plasmids**

Khoa Chung and Michael J. Booth*



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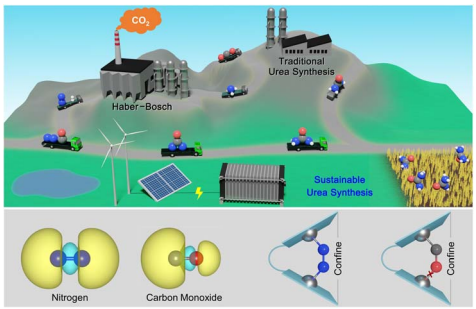
## EDGE ARTICLES

12707

**Steering competitive $N_2$ and CO adsorption toward efficient urea production with a confined dual site**

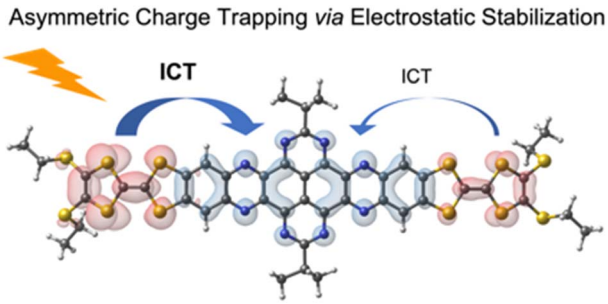
Zhe Chen, Yonghua Liu and Tao Wang*




12715

**Photoinduced asymmetric charge trapping in a symmetric tetraazapyrene-fused bis(tetrathiafulvalene) conjugate**

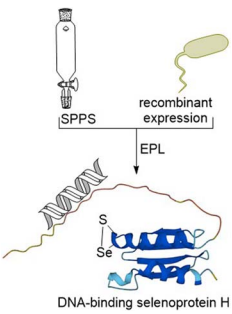
Ping Zhou, Maryam Nazari Haghighi Pashaki, Hans-Martin Frey, Andreas Hauser, Silvio Decurtins, Andrea Cannizzo,* Thomas Feurer, Robert Häner, Ulrich Aschauer* and Shi-Xia Liu*




12723

**The semisynthesis of nucleolar human selenoprotein H**

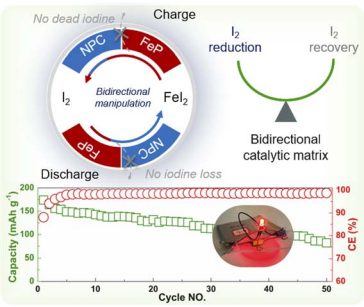
Rebecca Notis Dardashti, Shay Laps, Jacob S. Gichtin and Norman Metanis*




12730

**Bidirectional manipulation of iodine redox kinetics in aqueous Fe–$I_2$ electrochemistry**

Weiwei Zhang, Mingli Wang, Hong Zhang,* Lin Fu, Wenli Zhang, Yupeng Yuan* and Ke Lu*



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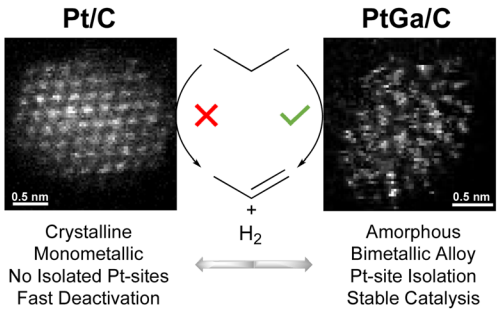
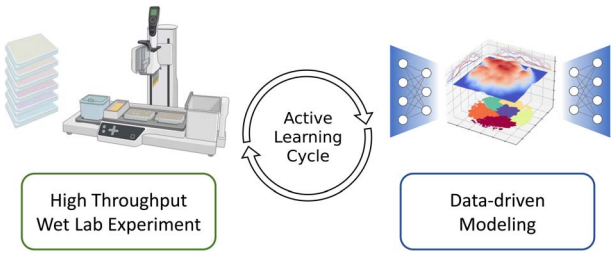
12739




**Implications of Ga promotion and metal–oxide interface from tailored PtGa propane dehydrogenation catalysts supported on carbon**

Enzo Brack, Milivoj Plodinec, Marc-Georg Willinger and Christophe Copéret*

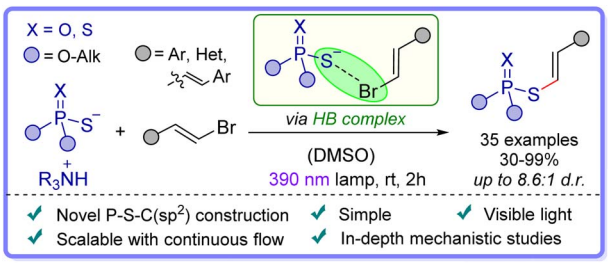
12747




**Data-driven discovery of innate immunomodulators *via* machine learning-guided high throughput screening**

Yifeng Tang, Jeremiah Y. Kim, Carman K. M. IP, Azadeh Bahmani, Qing Chen, Matthew G. Rosenberger, Aaron P. Esser-Kahn* and Andrew L. Ferguson*

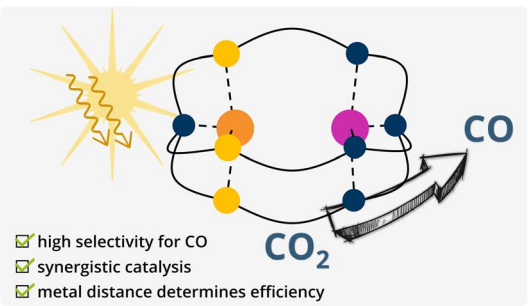
12767




**Photochemical halogen-bonding assisted carbothiophosphorylation reactions of alkenyl and 1,3-dienyl bromides**

Helena F. Piedra, Victoria Gebler, Carlos Valdés and Manuel Plaza*

12774




**A $Cu^{I}Co^{II}$ cryptate for the visible light-driven reduction of $CO_2$**

Julia Jökel, Esma Birsen Boydas, Joël Wellauer, Oliver S. Wenger, Marc Robert, Michael Römelt* and Ulf-Peter Apfel*



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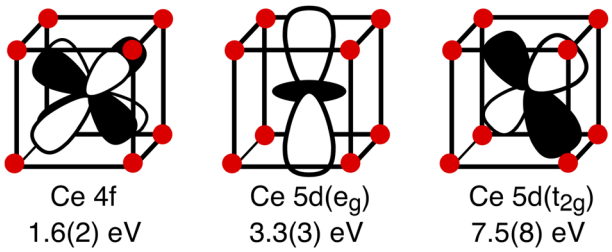
12784

**Strengths of covalent bonds in $LnO_2$ determined from O K-edge XANES spectra using a Hubbard model**

Wayne W. Lukens, Jr,* Stefan G. Minasian and Corwin H. Booth




## CORRECTION

12796

**Correction: Fast and scalable solvent-free access to Lappert's heavier tetrylenes $E\{N(SiMe_3)_2\}_2$ (E = Ge, Sn, Pb) and $ECl\{N(SiMe_3)_2\}$ (E = Ge, Sn)**

Javier A. Cabeza, Javier F. Reynes, Felipe García,* Pablo García-Álvarez* and Rubén García-Soriano