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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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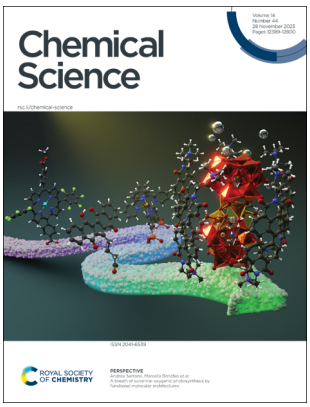

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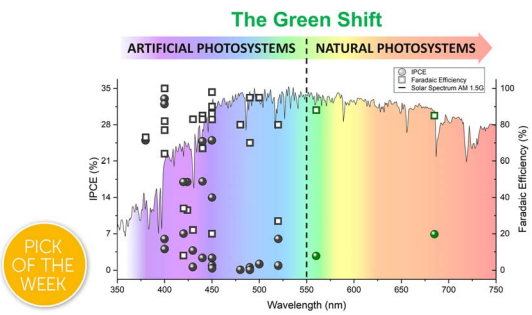
See Andrea Sartorel, Marcella Bonchio *et al.*, pp. 12402–12429. Image reproduced by permission of Marcella Bonchio from *Chem. Sci.*, 2023, **14**, 12402. Robin N. Dürr is thankfully acknowledged for designing and creating the cover artwork.

PERSPECTIVES

12402

A breath of sunshine: oxygenic photosynthesis by functional molecular architectures

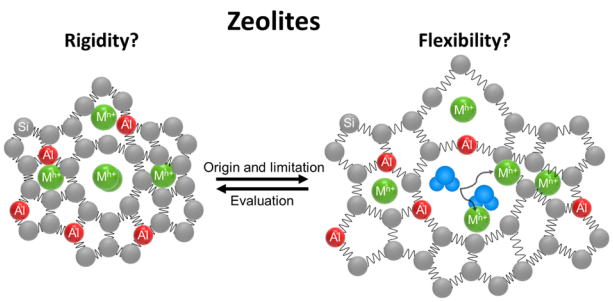
Thomas Gobbato, Giulia Alice Volpato, Andrea Sartorel* and Marcella Bonchio*



12430

Flexibility in zeolites: origin, limits, and evaluation

Sajjad Ghojavand, Eddy Dib and Svetlana Mintova*



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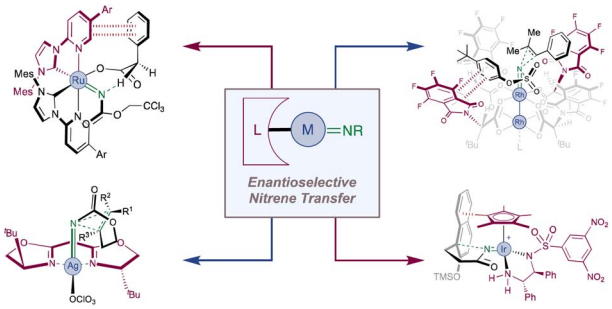
REVIEW

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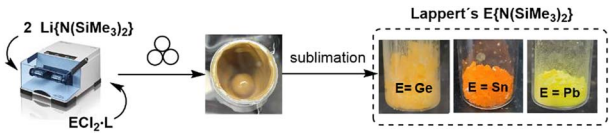
Fast and scalable solvent-free access to Lappert's heavier tetrylenes $E\{N(SiMe_3)_2\}_2$ (E = Ge, Sn, Pb) and $ECl\{N(SiMe_3)_2\}$ (E = Ge, Sn)

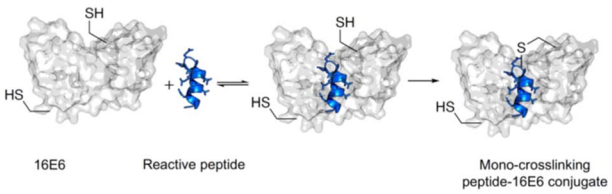
Javier A. Cabeza, Javier F. Reynes, Felipe García,* Pablo García-Álvarez* and Rubén García-Soriano



12484

Discovery of reactive peptide inhibitors of human papillomavirus oncoprotein E6

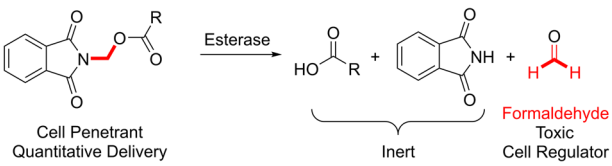
Xiyun Ye, Peiyuan Zhang, Jason Tao, John C. K. Wang, Amirhossein Mafi, Nathalie M. Grob, Anthony J. Quartararo, Hannah T. Baddock, Leanne J. G. Chan, Fiona E. McAllister, Ian Foe, Andrei Loas, Dan L. Eaton, Qi Hao, Aaron H. Nile* and Bradley L. Pentelute*



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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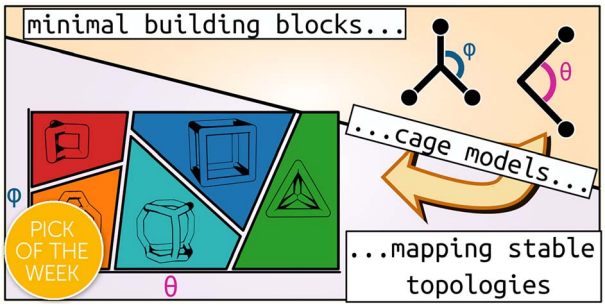
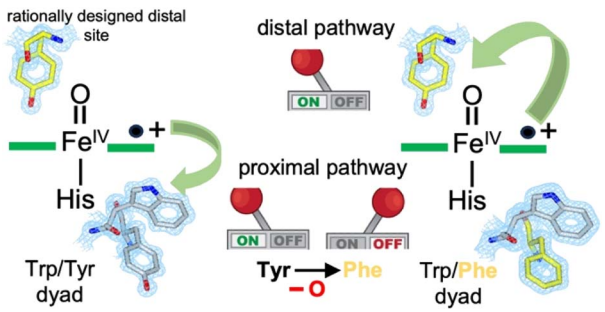


Systematic exploration of accessible topologies of cage molecules *via* minimalistic models

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

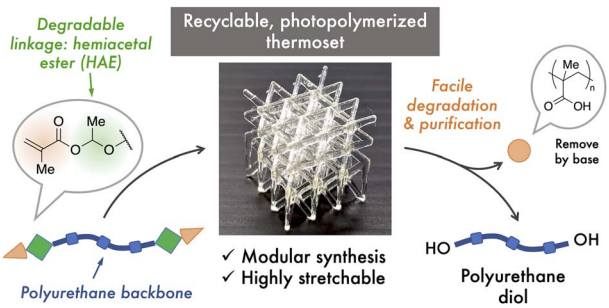
12518



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*

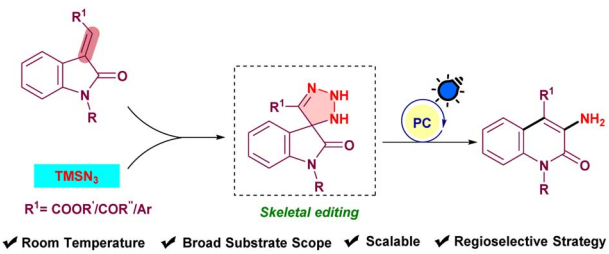
12535



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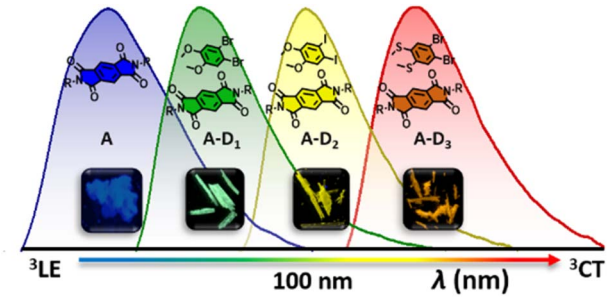
Revisiting organic charge-transfer cocrystals for wide-range tunable, ambient phosphorescence

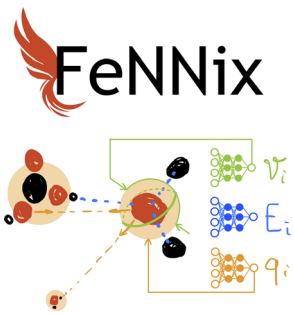
Anju Ajayan Kongasseri, Shagufi Naz Ansari, Swadhin Garain, Sopan M. Wagalgave and Subi J. George*



12554

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

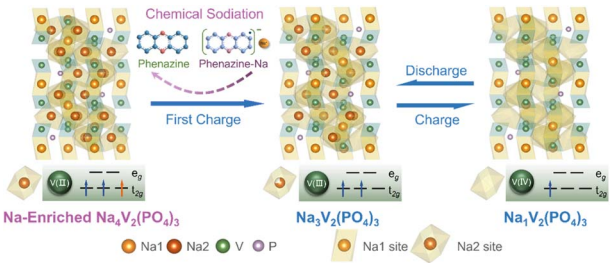
Thomas Plé,* Louis Lagardère* and Jean-Philip Piquemal*



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*



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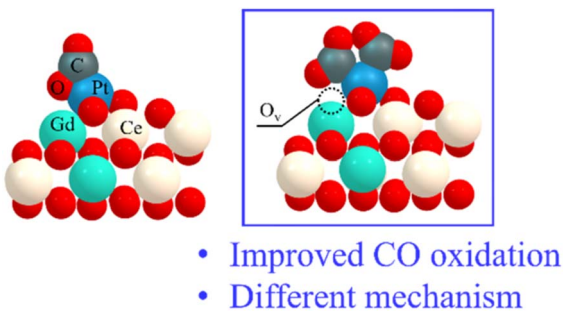
Active sites of atomically dispersed Pt supported on Gd-doped ceria with improved low temperature performance for CO oxidation

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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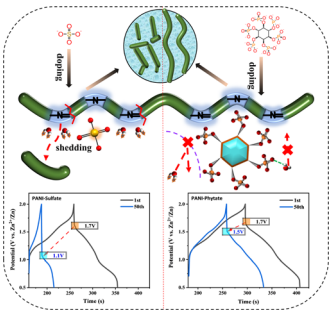
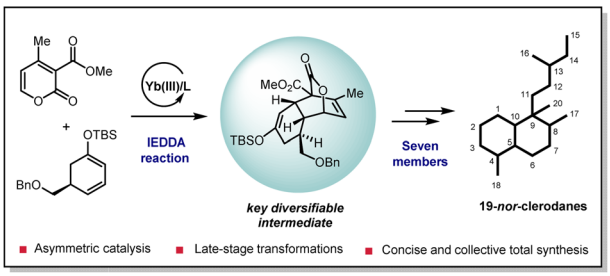


Enhancing organic cathodes of aqueous zinc-ion batteries *via* utilizing steric hindrance and electron cloud equalization

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*

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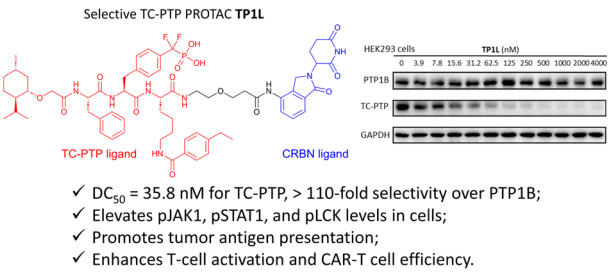

Discovery of a selective TC-PTP degrader for cancer immunotherapy

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*

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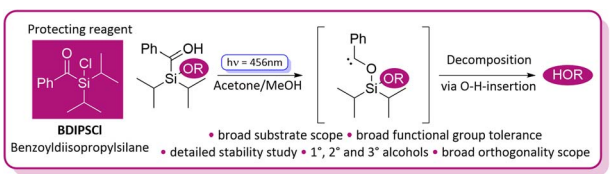

Benzoyldiisopropylchlorosilane: a visible light photocleavable alcohol protecting group

Florian Lind, Kirill Markelov and Armido Studer*

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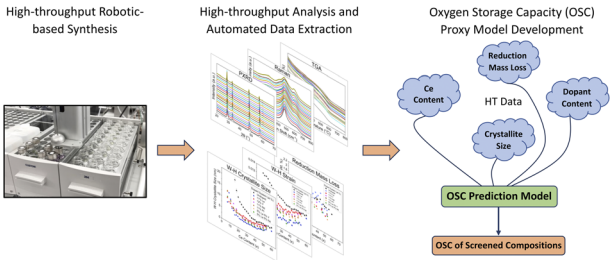
12621

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*

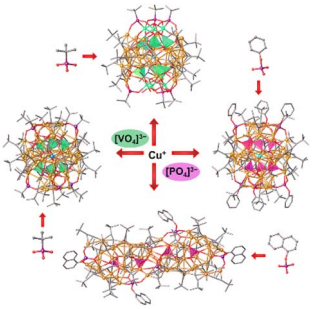


Accelerated discovery of high OSC Materials through high-throughput synthesis, analysis, and proxy models.

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*



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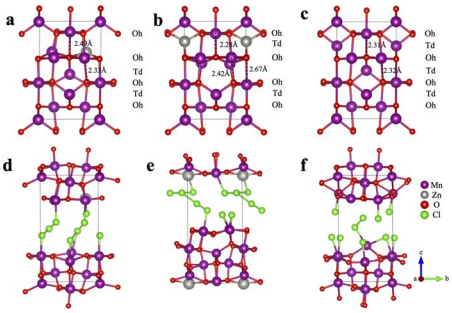
Reversible Cl/Cl⁻ redox in a spinel Mn_3O_4 electrode

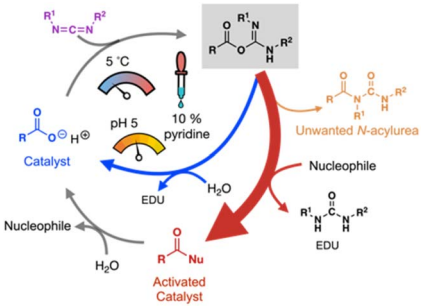
Sean K. Sandstrom, Qiuyao Li, Yiming Sui, Mason Lyons, Chun-Wai Chang, Rui Zhang, Heng Jiang, Mingliang Yu, David Hoang, William F. Stickle, Huolin L. Xin,* Zhenxing Feng,* De-en Jiang* and Xiulei Ji*



12653

Suppressing catalyst poisoning in the carbodiimide-fueled reaction cycle

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



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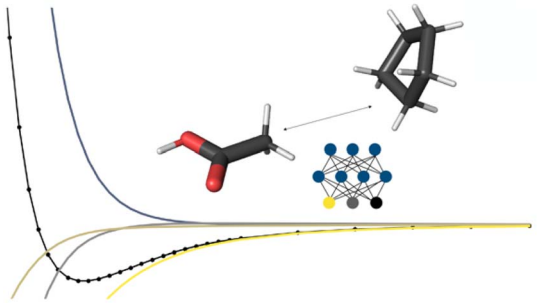
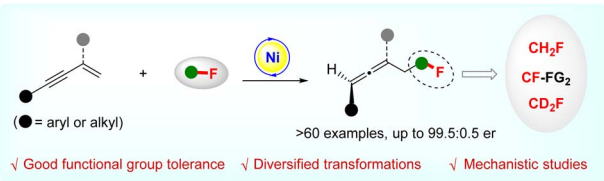
12661



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

Moritz Thürlemann and Sereina Riniker*

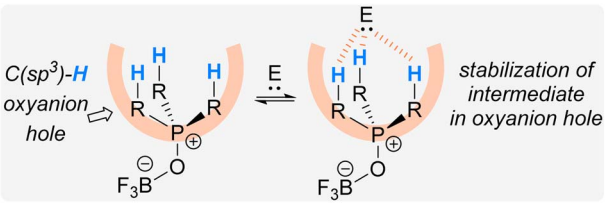
12676



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*

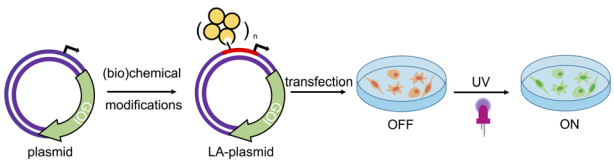
12684



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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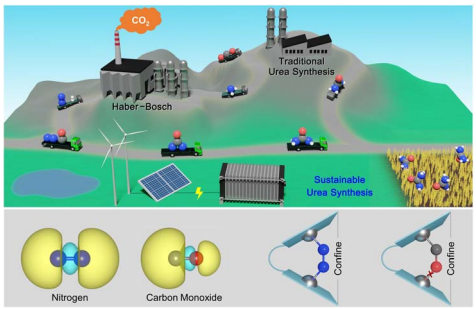
12707

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

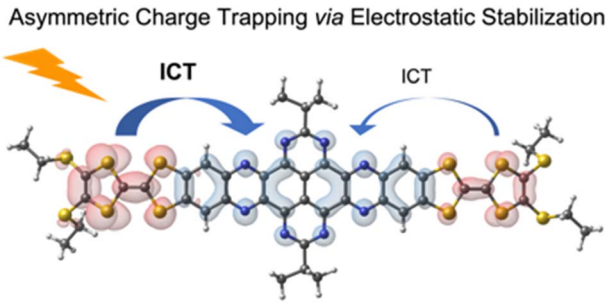
Zhe Chen, Yonghua Liu and Tao Wang*



12715

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

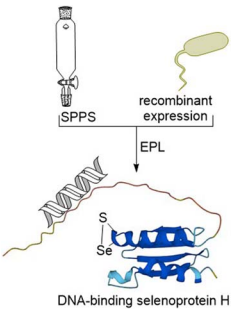
Ping Zhou, Maryam Nazari Haghighi Pashaki, Hans-Martin Frey, Andreas Hauser, Silvio Decurtins, Andrea Cannizzo,* Thomas Feurer, Robert Häner, Ulrich Aschauer* and Shi-Xia Liu*



12723

The semisynthesis of nucleolar human selenoprotein H

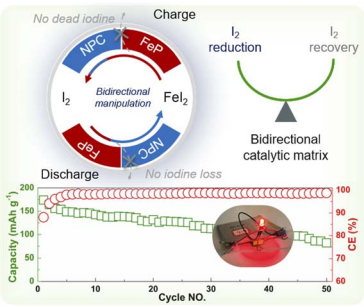
Rebecca Notis Dardashti, Shay Laps, Jacob S. Gichtin and Norman Metanis*



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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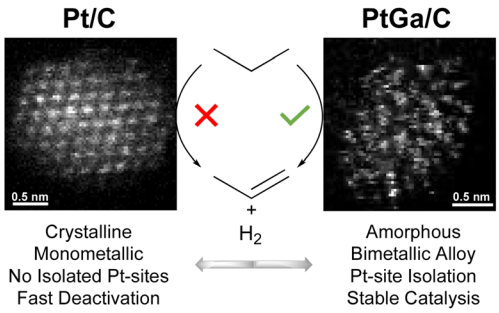
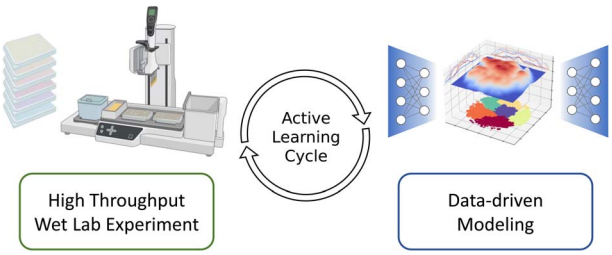
12739



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*

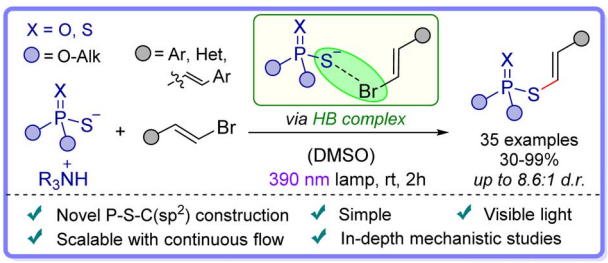
12747



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*

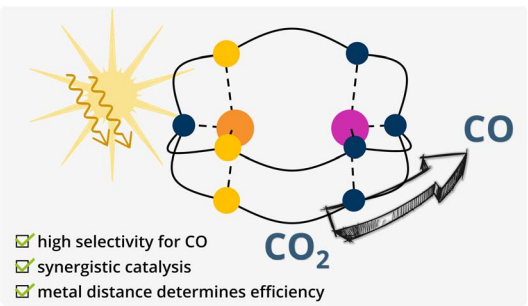
12767



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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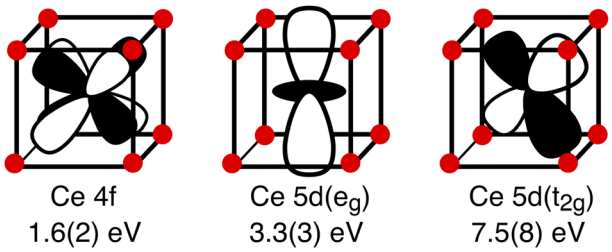
12784

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