

IN THIS ISSUE

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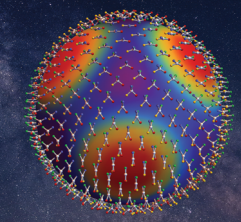
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ROYAL SOCIETY OF CHEMISTRY

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Chemical Science

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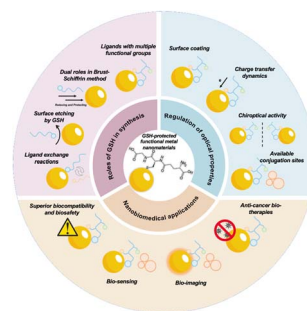
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Inside cover
See Peter J. Canfield and
Maxwell J. Crossley,
pp. 6705–6719. Image
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J. Crossley from *Chem. Sci.*,
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6542

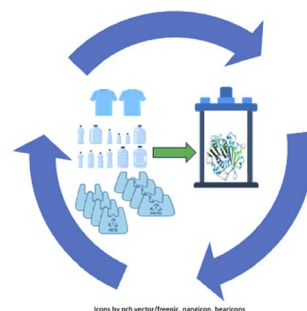
Zhucheng Yang, Jingkuan Lyu, Jing Qian, Yifan Wang,
Zhenghan Liu, Qiaofeng Yao, Tiankai Chen,* Yitao Cao*
and Jianping Xie*



6573

Biocatalytic recycling of plastics: facts and fiction

Wolfgang Zimmermann



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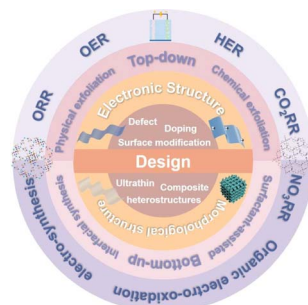


REVIEWS

6583

Two-dimensional metal organic framework nanosheets in electrocatalysis

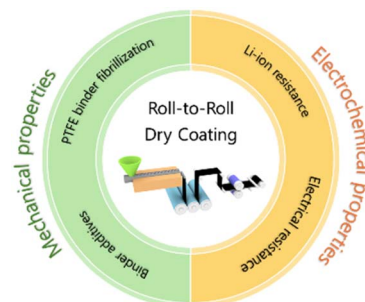
Ping Wang, Cheng Yang, Jiasai Yao, Huawei Li, Zikang Hu and Zhenxing Li*



6598

Sustainable and cost-effective electrode manufacturing for advanced lithium batteries: the roll-to-roll dry coating process

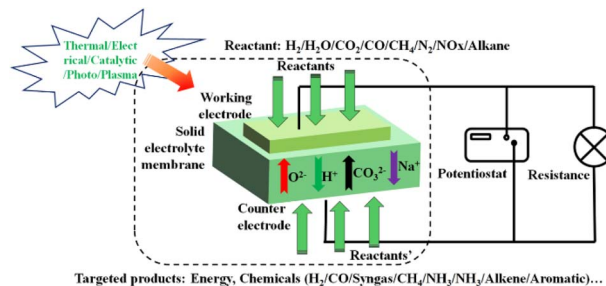
Joonhyeok Park, Jiwoon Kim, Jaeik Kim, Minsung Kim, Taeseup Song* and Ungyu Paik*



6620

Status and outlook of solid electrolyte membrane reactors for energy, chemical, and environmental applications

Liangdong Fan,* Wanying Luo, Qixun Fan, Qicheng Hu, Yifu Jing, Te-Wei Chiu* and Peter D. Lund*

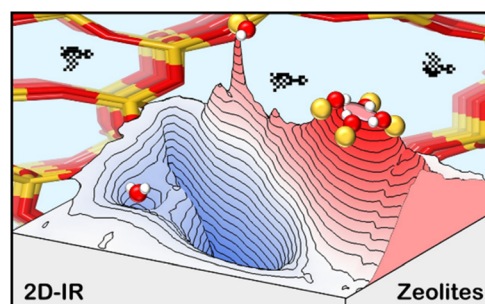


EDGE ARTICLES

6688

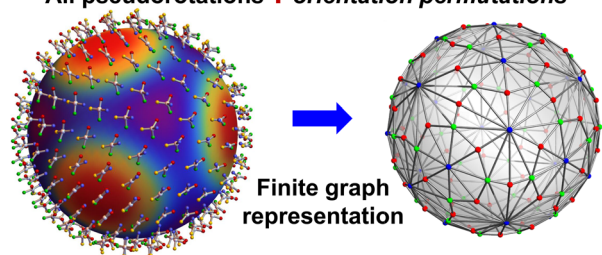
Distinctive signatures and ultrafast dynamics of Brønsted sites, silanol nests and adsorbed water in zeolites revealed by 2D-IR spectroscopy

Paul M. Donaldson,* Alexander P. Hawkins and Russell F. Howe



6705

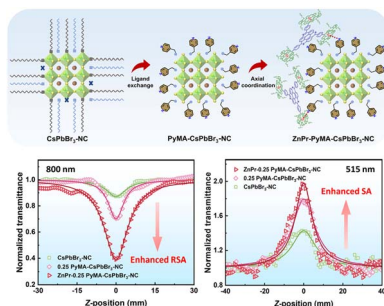
Full AB_n configuration spaces All pseudorotations + orientation permutations



Rigorous treatment of polytopal rearrangements reveal surprising complexity of stereoisomerism configuration landscapes

Peter J. Canfield* and Maxwell J. Crossley*

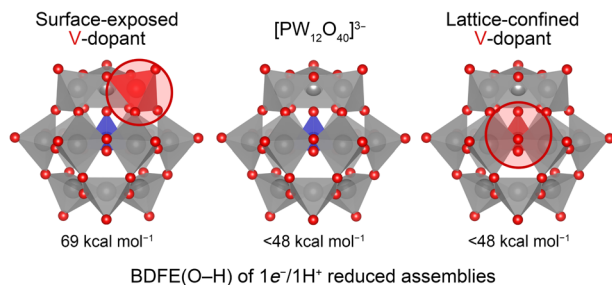
6720



Greatly enhanced ultrafast optical absorption nonlinearities of pyridyl perovskite nanocrystals axially modified by star-shaped porphyrins

Zihao Guan, Lulu Fu, Lu Chen, Zhiyuan Wei, Fang Liu, Yang Zhao, Zhipeng Huang, Mark G. Humphrey and Chi Zhang*

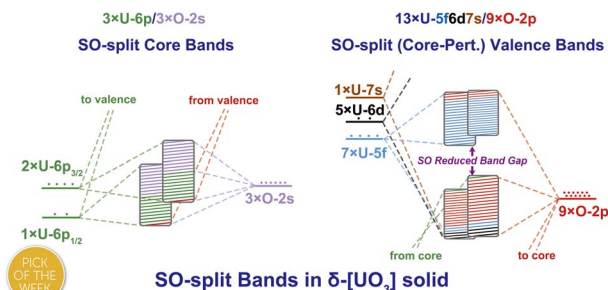
6736



Location of dopant dictates proton-coupled electron transfer mechanism in vanadium-substituted polyoxotungstates

Zhou Lu, Mamta Dagar, James R. McKone and Ellen M. Matson*

6744



Valence activity of SO-coupled atomic core shells in solid compounds of heavy elements

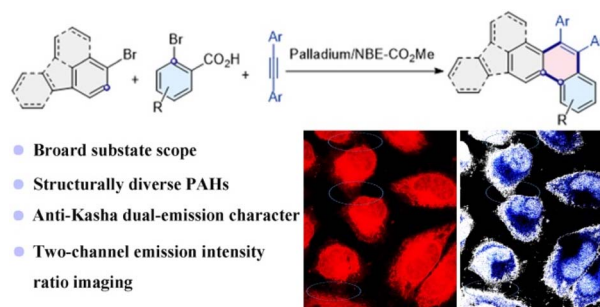
Shi-Ru Wei, Han-Shi Hu, W. H. Eugen Schwarz* and Jun Li*



6755

Palladium/norbornene-catalyzed C–H bond activation and annulation to construct polycyclic aromatic hydrocarbon-based fluorescent materials

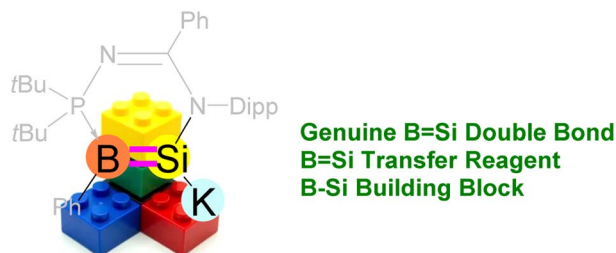
Chunlin Zhou, Xianhui Yang, Lian Gou and Bijin Li*



6763

An *N*-phosphinoamidinato borasilenide: a vinyl-analogous anion containing a base-stabilised B=Si double bond

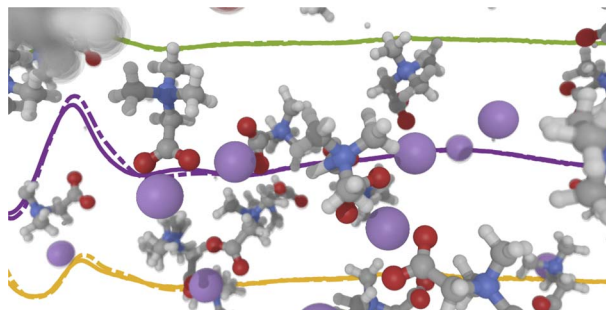
Si Jia Isabel Phang, Zheng-Feng Zhang, Ming-Der Su* and Cheuk-Wai So*



6770

Specific ion effects enhance local structure in zwitterionic osmolyte solutions

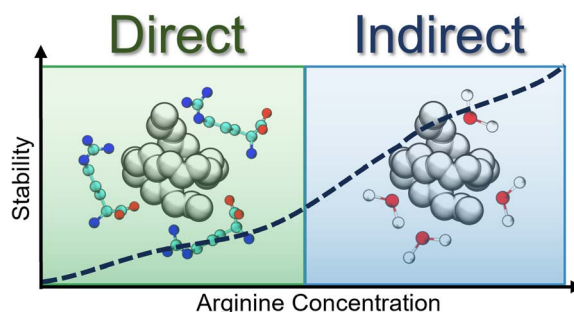
Kieran J. Agg, Timothy S. Groves, Shurui Miao, Y. K. Catherine Fung, Oliver L. G. Alderman, Thomas F. Headen, Terri-Louise Hughes, Gregory N. Smith, Tristan G. A. Youngs, James P. Tellam, Yao Chen, Susan Perkin and James E. Hallett*



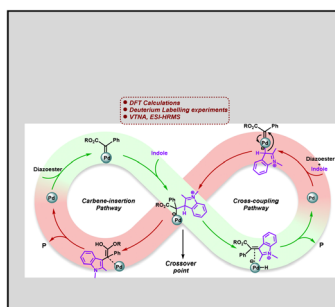
6780

Flipping out: role of arginine in hydrophobic interactions and biological formulation design

Jonathan W. P. Zajac, Praveen Muralikrishnan, Idris Tohidian, Xianci Zeng, Caryn L. Heldt, Sarah L. Perry and Sapna Sarupria*



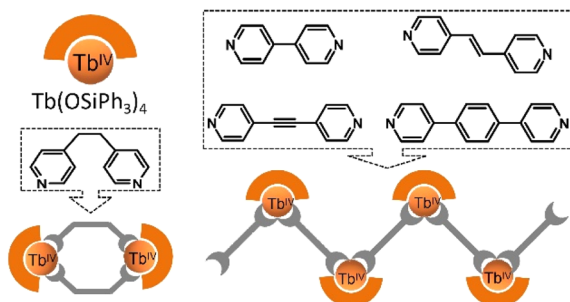
6793



A combined experimental and computational study reveals a crossover between conventional cross-coupling and carbene insertion pathways in a Pd catalyzed C(sp²)-H insertion

Arushi Tyagi, Kritika Gaur, Anubhav Goswami, Arko Seal, Mayuk Joddar and Garima Jindal*

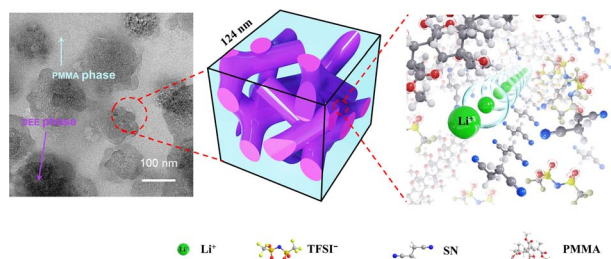
6805



Supramolecular assemblies of tetravalent terbium complex units: syntheses, structure, and materials properties

Tianjiao Xue, Qing-Song Yang, Lei Li, Xiao-Yong Chang, You-Song Ding* and Zhiping Zheng*

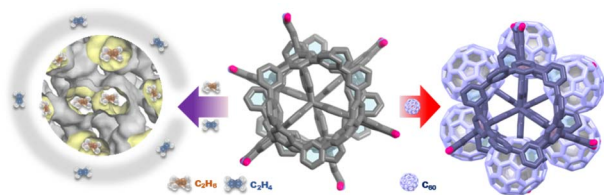
6812



Advancing lithium metal batteries with *in situ* polymerized PMMA-based elastomeric electrolytes

Zhengyin Yao, Zhen Liu, Kang Xia, Haoru Xie, Shiyan Xie and Peng Zhang*

6822



A triply linked propellane-nanoring hybrid serving as a good host

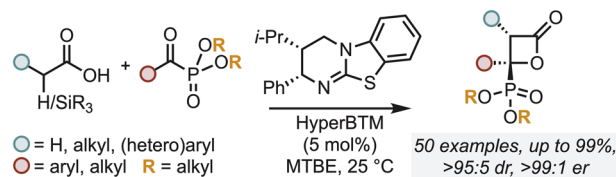
Yan Chen, Xingyu Chen, Lin Li, Xiangping Chen, Jianlong Xia and Lei Zhang*



6828

Isothiourea-catalysed enantioselective synthesis of phosphonate-functionalised β -lactones

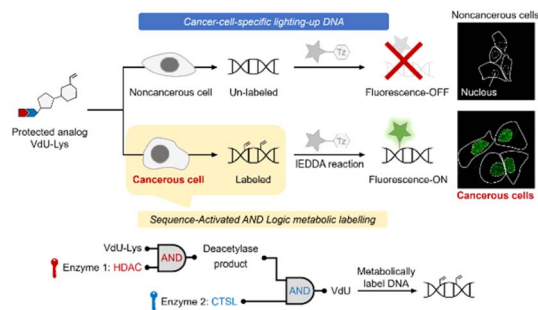
Ffion M. Platt, Yihong Wang, David B. Cordes, Aidan P. McKay, Alexandra M. Z. Slawin, Heena Panchal and Andrew D. Smith*



6837

Sequential metabolic probes illuminate nuclear DNA for discrimination of cancerous and normal cells

Caiqi Liu, Sirui Lu, Chenxu Yan,* Xingyuan Zhao, Jing Yang, Weixu Zhang, Xiuyan Zhao, Yao Ge, Xiaofan You and Zhiqian Guo*



6845

Atomic-level engineering of single Ag^{1+} site distribution on titanium-oxo cluster surfaces to boost CO_2 electroreduction

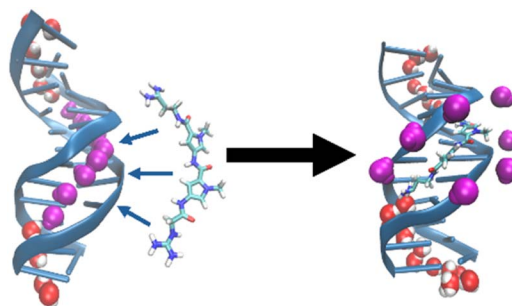
Ru-Xin Meng, Lan-Cheng Zhao, Li-Pan Luo, Yi-Qi Tian, Yong-Liang Shao, Qing Tang,* Likai Wang,* Jun Yan and Chao Liu*



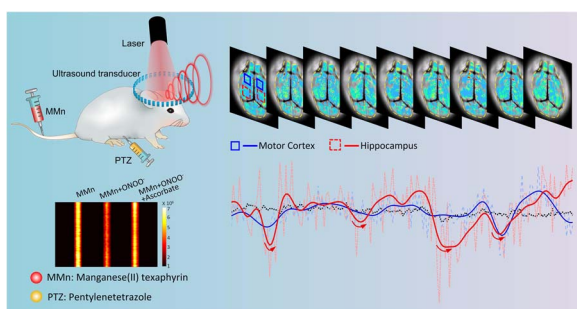
6853

Drug binding disrupts chiral water structures in the DNA first hydration shell

Ty Santiago, Daniel Konstantinovskiy, Matthew Tremblay, Ethan A. Perets,* Sharon Hammes-Schiffer* and Elsa C. Y. Yan*



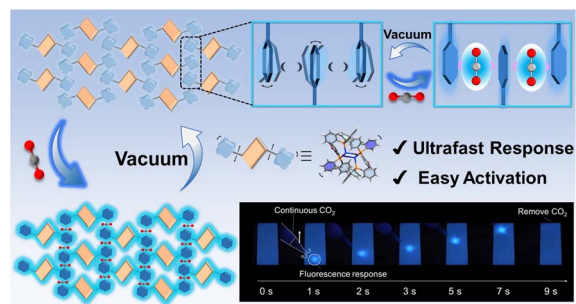
6862



Real-time visualization of epileptic seizures using photoacoustic imaging with a peroxynitrite-responsive manganese(II) texaphyrin

Yaguang Ren, Calvin V. Chau, Tao Chen, Jingqin Chen, Yu Hu, Zhonghua Lu, James T. Brewster, Jonathan F. Arambula, Rongkang Gao, Adam C. Sedgwick,* Jonathan L. Sessler* and Chengbo Liu*

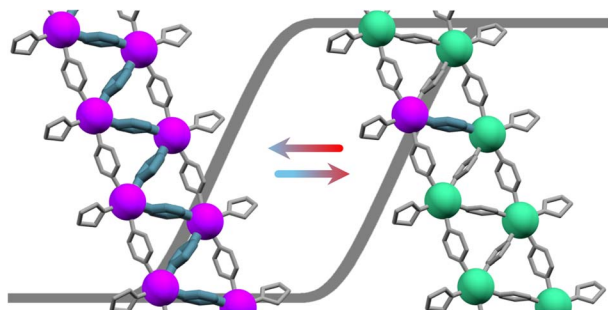
6872



CO₂-enhanced TADF of an ultra-stable Cu(I) cluster via guest–host π – π interaction

Hong-Jin Zhang, Zong-Ren Chen, Ji-Tong Xu, Jia-Wen Ye,* Ling Chen* and Xiao-Ming Chen

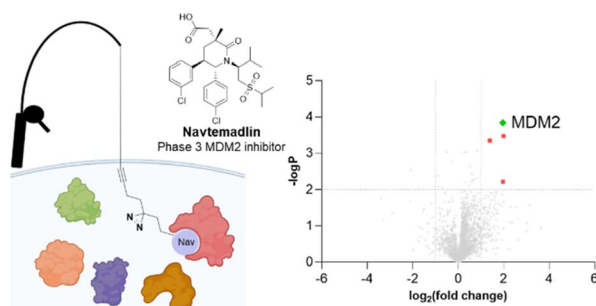
6879



Disentangling chemical pressure and superexchange effects in lanthanide–organic valence tautomerism

Anton Viborg, Maja A. Dunstan,* Nathan J. Yutronkie, Amit Chanda, Felix Trier, Nini Pryds, Fabrice Wilhelm, Andrei Rogalev, Dawid Pinkowicz and Kasper S. Pedersen*

6886



Affinity-based protein profiling of MDM2 inhibitor Navtemadlin

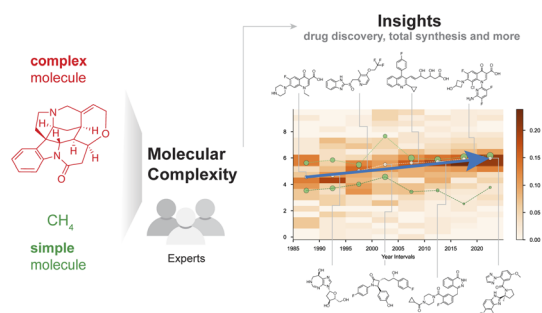
Amrita Date, Archie Wall, Peiyu Zhang, Jack W. Houghton, Jianan Lu, Adam M. Thomas, Tristan Kovačič, Andrew J. Wilson, Edward W. Tate and Anna Barnard*



6895

Digitization of molecular complexity with machine learning

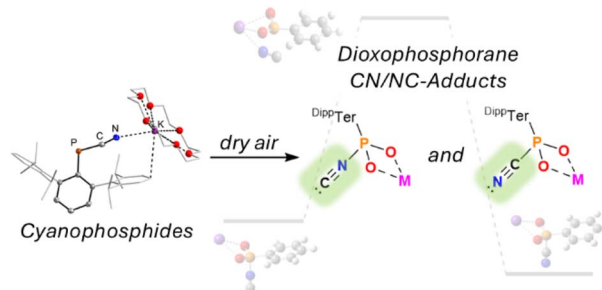
Andrei S. Tyrin, Daniil A. Boiko, Nikita I. Kolomoets and Valentine P. Ananikov*



6909

Coordination isomerism in dioxophosphorane cyanides

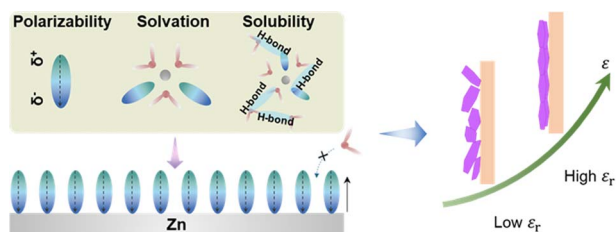
Ayu Afiah Nasrullah, Edgar Zander, Fabian Dankert, Andrey Petrov, Jonas Surkau, Eszter Baráth* and Christian Hering-Junghans*



6918

Anion-endowed high-dielectric water-deficient interface towards ultrastable Zn metal batteries

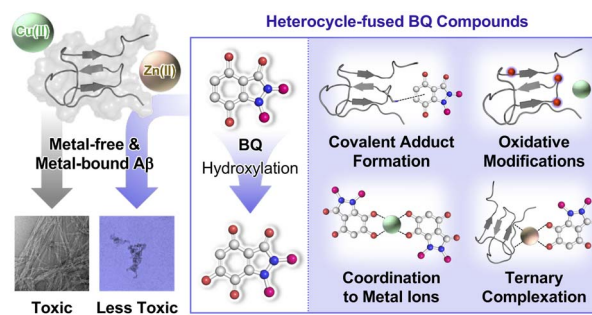
Xiangjie Liu, Xiaoxin Nie, Yujiao Yang, Meng Yao,* Jiaxian Zheng, Hanfeng Liang,* Mi Zhou, Jin Zhao, Yingqian Chen and Du Yuan*



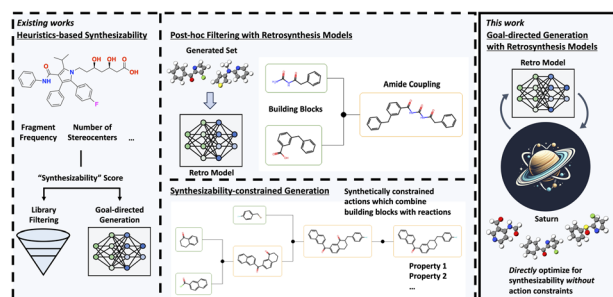
6930

Leveraging heterocycle-fused 1,4-benzoquinone to design chemical modulators for both metal-free and metal-bound amyloid-β

Yelim Yi, Kyungmin Kim, Hakwon Kim* and Mi Hee Lim*



6943

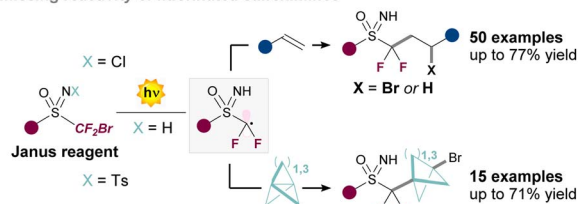


Directly optimizing for synthesizability in generative molecular design using retrosynthesis models

Jeff Guo* and Philippe Schwaller*

6957

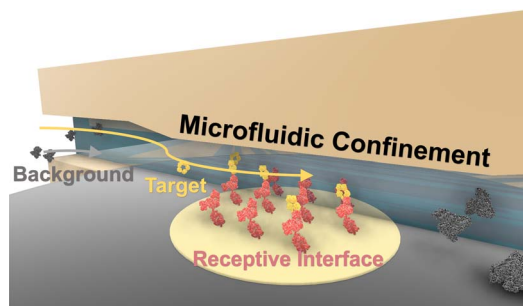
the missing reactivity of fluorinated sulfoximines



Radical photochemical difluorosulfoximation of alkenes and propellanes

Simone Baldon, Julien Paut, Elsa Anselmi, Guillaume Dagousset, Béatrice Tuccio, Giorgio Pelosi, Sara Cuadros,* Emmanuel Magnier* and Luca Dell'Amico*

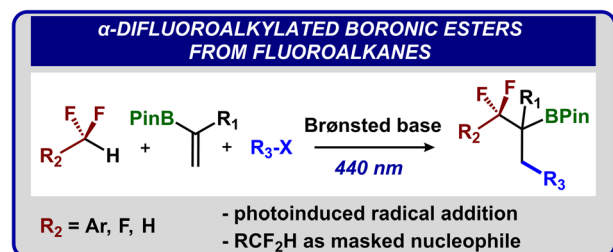
6965



Leveraging microfluidic confinement to boost assay sensitivity and selectivity

Shaoyu Kang and Jason J. Davis*

6975



Diversifying fluoroalkanes: light-driven fluoroalkyl transfer via vinylboronate esters

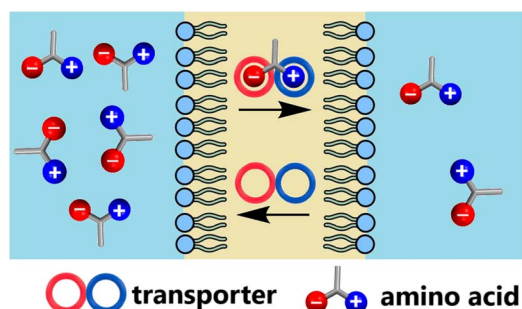
Kaushik Chakrabarti, Chandana Sunil, Benjamin M. Farris, Simon Berritt, Kyle Cassaidy, Jisun Lee and Nathaniel K. Szymczak*



6982

Squaramide-based ion pair receptors can facilitate transmembrane transport of KCl and zwitterions including highly polar amino acids

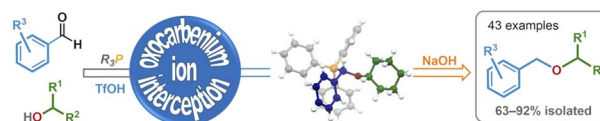
Marta Zaleskaya-Hernik, Rayhanus Salam, Mario J. González, Marcin Wilczek, Łukasz Dobrzycki, Nathalie Busschaert* and Jan Romański*



6991

Direct synthesis of ethers from alcohols & aldehydes enabled by an oxocarbenium ion interception strategy

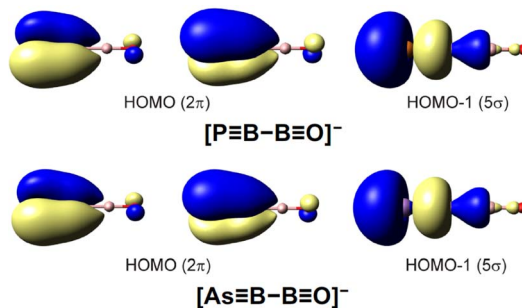
Dara T. Curran, Marcin Szydło, Helge Müller-Bunz, Kirill Nikitin* and Peter A. Byrne*



7004

$P\equiv B$ and $As\equiv B$ triple bonds in the linear PB_2O^- and AsB_2O^- species

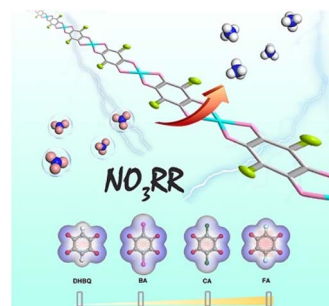
Han-Wen Gao, Jie Hui and Lai-Sheng Wang*



7010

Molecular engineering of 1D conjugated copper anilate coordination polymers for boosting electrocatalytic nitrate reduction to ammonia

Zhanning Liu,* Chengyong Xing, Yufei Shan, Min Ma, Shaowen Wu, Ruixiang Ge, Qingzhong Xue* and Jian Tian*



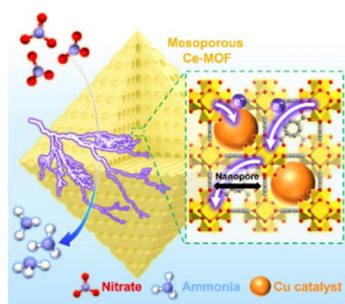
7018



Development of bright NIR-emitting pressure-sensitive paints using benzoporphyrin luminophores

Elliott J. Nunn,^{*} Dimitrios Tsioumanis, Tom B. Fisher, David A. Roberts, Mark K. Quinn^{*} and Louise S. Natrajan^{*}

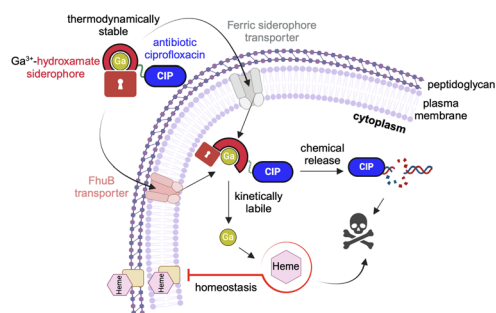
7026



Unlocking coordination sites of metal–organic frameworks for high-density and accessible copper nanoparticles toward electrochemical nitrate reduction to ammonia

Cheng-Hui Shen, Yingji Zhao,^{*} Ho Ngoc Nam, Liyang Zhu, Quan Manh Phung, Vic Austen, Minjun Kim, Dong Jiang, Xiaoqian Wei, Tokihiko Yokoshima, Chung-Wei Kung^{*} and Yusuke Yamauchi^{*}

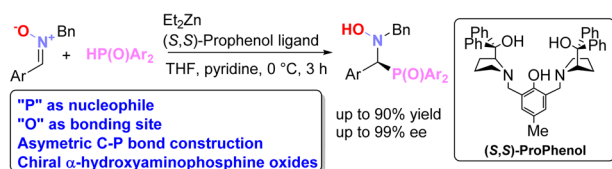
7039



Decoding growth inhibitory associated pathways of xenometal–siderophore antibiotic conjugates in *S. aureus*

Axia Marlin,^{*} Minhua Cao, Joelle El Hamouche, Owen Glaser and Eszter Boros^{*}

7051



Enantioselective Zn-catalyzed hydrophosphinylation of nitrones: an efficient approach for constructing chiral α -hydroxyamino-phosphine oxides

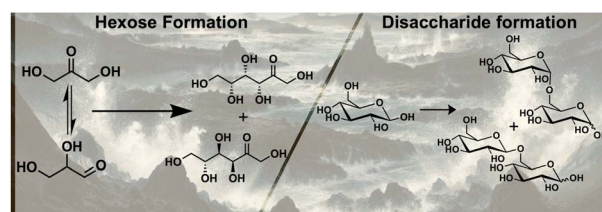
Shihui Luo, Xinzhu Yuan, Jiangtao Cheng, Zhiping Yang, Zhongxing Huang and Jun (Joelle) Wang^{*}



7057

Abiotic formation of hexoses and disaccharides in aqueous microdroplets

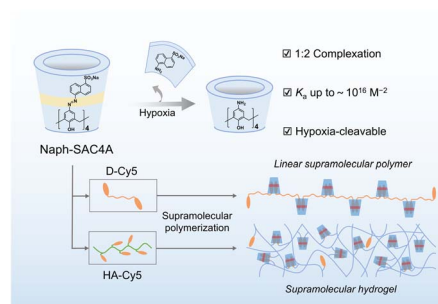
Myles Quinn Edwards, Dylan T. Holden and R. Graham Cooks*



7066

High-affinity 1 : 2 recognition based on naphthyl-azocalix[4]arene and its application as a cleavable noncovalent connector in constructing responsive supramolecular polymeric materials

Shun-Yu Yao, An-Kang Ying, Wen-Chao Geng, Fang-Yuan Chen, Xin-Yue Hu, Kang Cai* and Dong-Sheng Guo*



7077

An intramolecularly locked single molecule nanofluorophore with 13.55% quantum yield for SWIR multimodal phototheranostics

Leilei Si, Jun Tang, Kaixin Yang, Mingda Wang, Yigang Wang, Guomin Xia* and Hongming Wang*

