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IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 16(48) 22783–23410 (2025)

Cover
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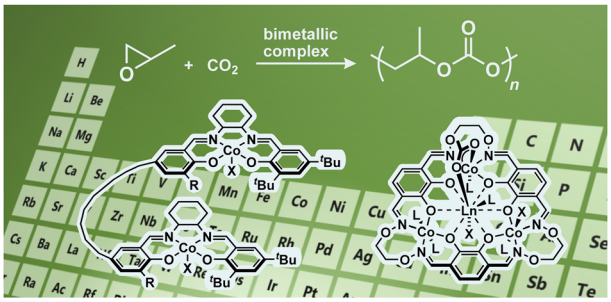
COMMENTARY

22801

A reflection on 'Bimetallic mechanism operating in the copolymerization of propylene oxide with carbon dioxide catalyzed by cobalt–salen complexes'

Koji Nakano* and Kyoko Nozaki*

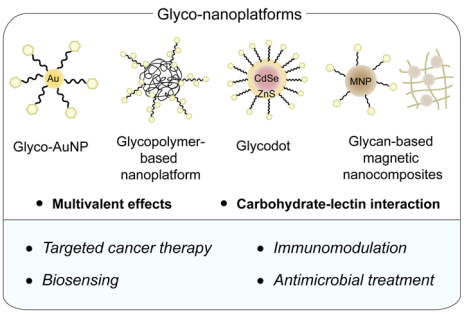


PERSPECTIVE

22805

Multivalently engineered glyco-nanoplatforms for targeted therapy and diagnostics

Xiao-Lin Zhang, Han Ding, Jia-Yi Zheng, Hongzhi Cao and Xue-Wei Liu*



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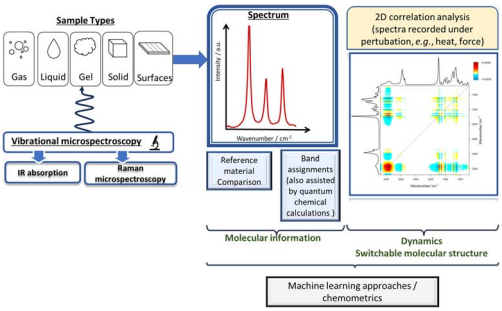
REVIEWS

22826

Label-free linear and non-linear vibrational spectroscopy for functional materials: state-of-the-art and future perspectives

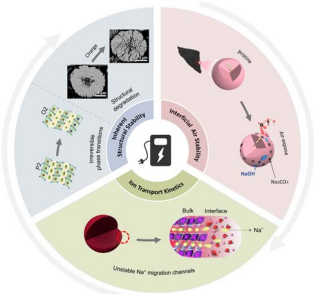
Michael Freduah Agyemang,* Akuila L. J. L. Edwards, Stefan Zechel, Martin D. Hager, Michael Schmitt and Juergen Popp



22852

Lattice-coherent interface-reinforced sodium-layered oxide cathodes

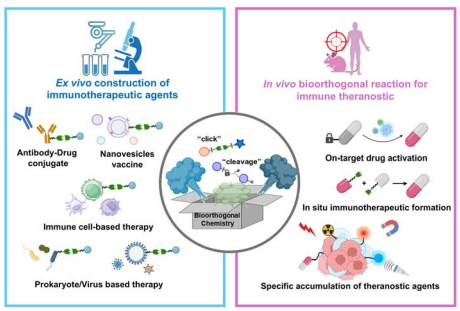
Sun-Qi Su, Qi-Cong Ling, Yan-Jiang Li,* Ya-Ping Yan,* Yan-Fang Zhu* and Yao Xiao*



22870

A powerful bioorthogonal toolbox boosting the development of immune theranostics

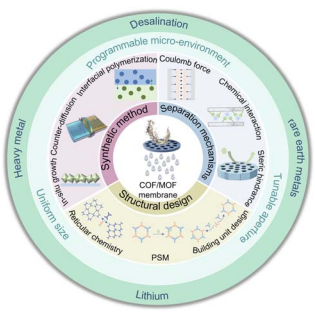
Songhan Liu, Chenyu Hua, Xianan Li, Pengcheng Yuan and Bengang Xing*



22900

Covalent/metal–organic framework membranes with tailored pore functionality for accurate ion separation

Penglin Cheng, Tiantian Chen, Tiantian Liu, Yuhan Wei, Miaomiao Tian,* Xueli Cao, Shi-Peng Sun, Yatao Zhang, Bart Van der Bruggen and Junyong Zhu*



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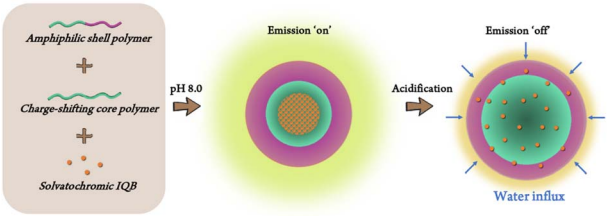
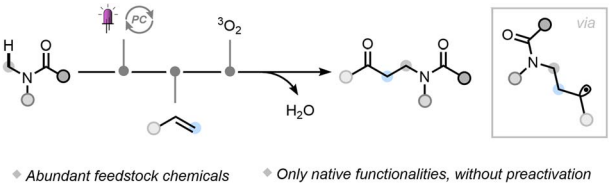


Monitoring structural change and drug release of responsive nanoparticles using polarity-sensitive fluorophores

Yanting Gao, Peter W. McDonald, Chris Ritchie* and Georgina K. Such*

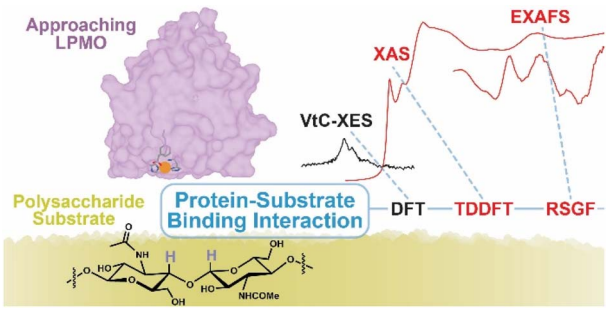
22944



Photocatalyzed hydrogen atom transfer enables multicomponent olefin oxo-amidomethylation under aerobic conditions

Mattia Lepori, Dimitris I. Ioannou, Joshua P. Barham* and Timothy Noël*

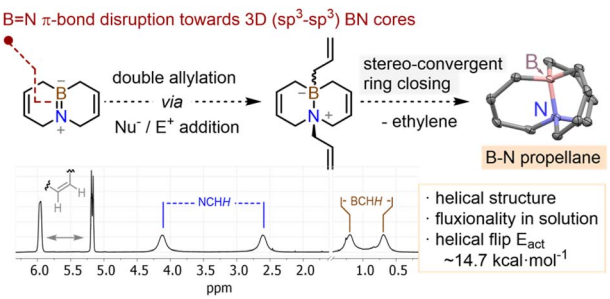
22952



Structural and electronic modulations of lytic polysaccharide monooxygenase (LPMO) upon chitin binding: insights from X-ray spectroscopy

Chris Joseph, Ashish Tamhankar, Ole Golten, Kushal Sengupta, Sergio A. V. Jannuzzi, Morten Sørlie, Liqun Kang, Åsmund K. Røhr, Vincent G. H. Eijsink* and Serena DeBeer*

22970



B–N axis as a facilitating agent for the synthesis of 3D structures: the paradigmatic case of BN-[4.4.4] propellane

Guillem Sanz-Liarte, Josep Saurí, Pau Nolis, Ana B. Cuenca* and Alexandr Shafir*

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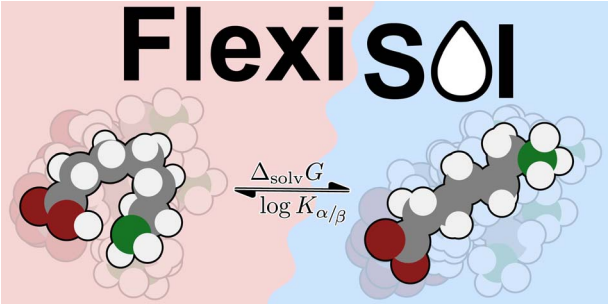
A diverse and chemically relevant solvation model benchmark set with flexible molecules and conformer ensembles

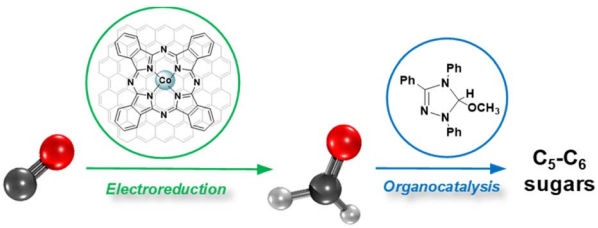
Lukas Wittmann, Christian Erik Selzer and Stefan Grimme*



22996

CO-to-sugars conversion from one-pot two-step electro-organocatalytic process

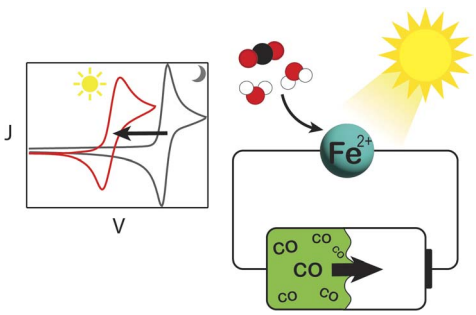
Ajeet Singh, David Martins-Bessa, Julien Bonin,* Marc Robert* and Sébastien Bontemps*



23005

Photosynthesis of CO from CO_2 with an iron polypyridyl catalyst at a passivated silicon photoelectrode

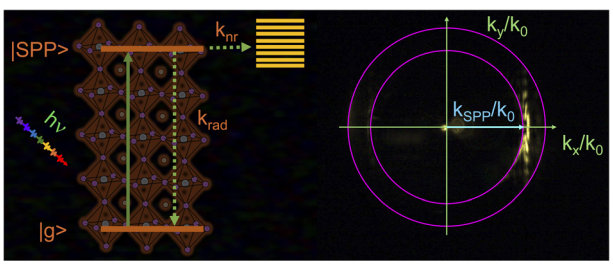
Gabriella P. Bein, Sergio Fernández, Stephen J. Tereniak, Renato N. Sampaio, Alexander J. M. Miller* and Jillian L. Dempsey*



23012

Energy transfer and radiation damping in gold–$MAPbI_3$ heterostructures

Bikram Ghosh, Ajinkya Shingote, Janak Bhandari and Gregory V. Hartland*



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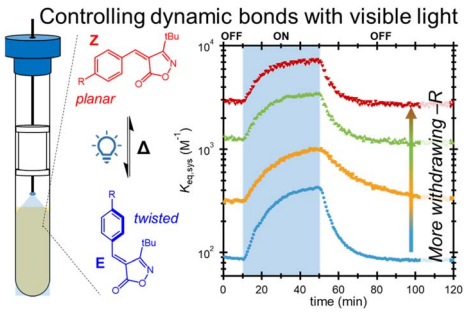
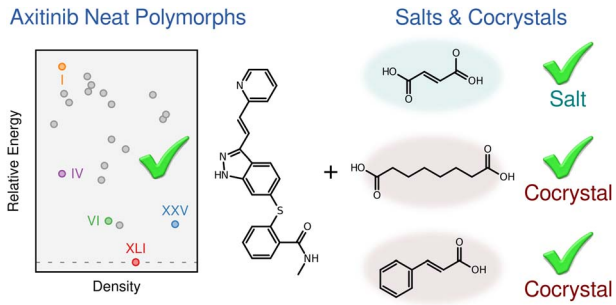


Manipulating dynamic covalent bonds through direct photoisomerization

Neil D. Dolinski,* Alex E. Crolais, Nicholas R. Boynton, Chuqiao Chen, Juan J. de Pablo, Scott A. Snyder* and Stuart J. Rowan*

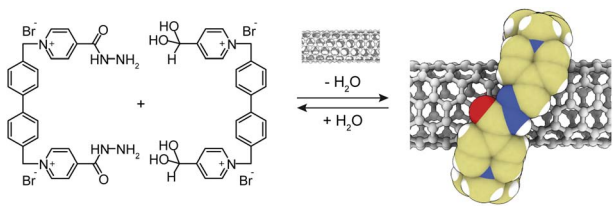
23026



From polymorphs to cocrystals and salts: successfully predicting axitinib's challenging crystal forms

Gregory J. O. Beran*

23038



Extended white-box cyclophanes for the synthesis of mechanically interlocked derivatives of single-walled carbon nanotubes in water

Julia Villalva, Arturo Blanco-Gómez, David M. Jiménez, Alejandro López-Moreno, M. Luisa Ruiz-González, Carlos Peinador,* Marcos D. García* and Emilio M. Pérez*

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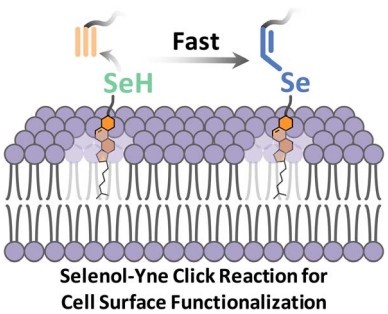

Efficient and rapid cell surface functionalization: a sub-minute selenol-yne click reaction for bioconjugation

Fangjian Shan, Xingyu Heng, Lihua Yao, Guichuan Xu, Jun Hu, Xiangqiang Pan* and Gaojian Chen*

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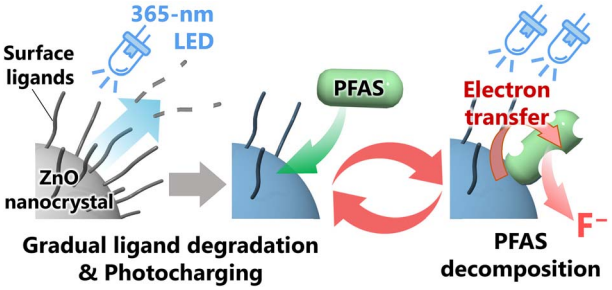
Photocatalytic defluorination of perfluoroalkyl substances by surface-engineered ZnO nanocrystals

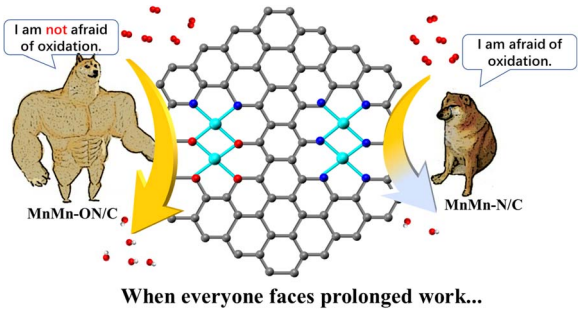
Shuhei Kanao, Mai Yamaguchi, Yuto Toyota, Yuki Nagai and Yoichi Kobayashi*



23064

A universal N_2O_4-cavity strategy for precisely spaced, durable dual-atom ORR catalysts

Guangxu Yao, Huijuan Zhang,* Yangjun Luo, Chuanzhen Feng and Yu Wang*



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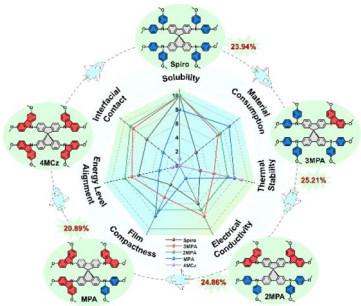
Rigid-flexible coupling: exquisite modulation of asymmetrical spiro-type hole-transporting materials toward efficient and stable perovskite solar cells

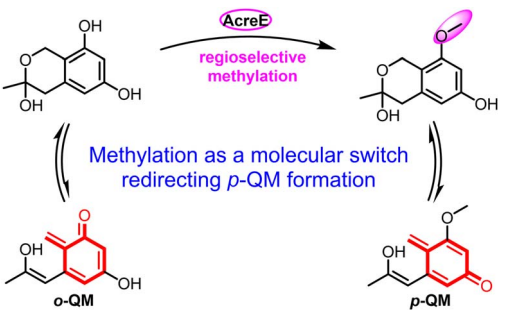
Xuran Wang, Jihong Wu, Guosen Zhang, Ruidan Zhang, Mingwei An,* Xiafeng He, Xiaozhen Huang, Jie Gao, Hongfang Du, Yue Wang, Dong Wei,* Daqin Chen,* Yang Wang* and Wei Huang*



23088

A methyltransferase molecular switch unlocks *para*-quinone methide generation and oligomerization

Chuanteng Ma, Zhenzhen Zhang, Wenxue Wang, Falei Zhang, Aowei Xie, Kaijin Zhang, Xingtao Ren, Lu Wang, Qian Che, Tianjiao Zhu, Junfeng Zhang* and Dehai Li*



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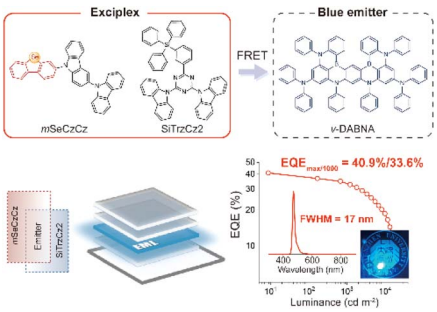
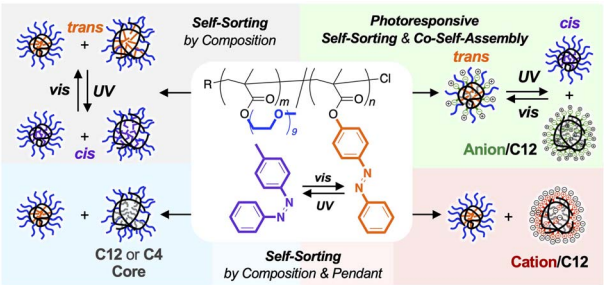


Exciplex spin-flip acceleration enables high-performance narrowband electroluminescence

Mengcheng Wang, Zhanxiang Chen,* Manli Huang, Dengke Wang, Cheng Zhong, Zheng-Hong Lu and Chuluo Yang*

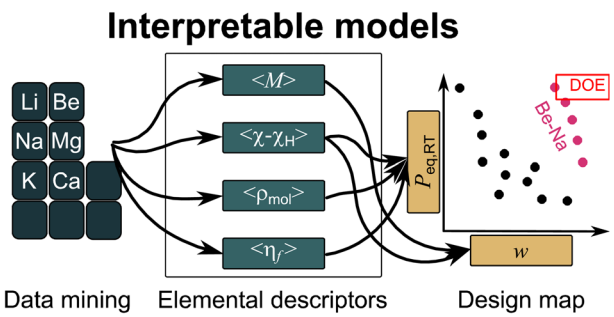
23103



Self-sorting systems of photoresponsive polymer micelles: isomerization drives reversible and switchable self-assembly

Rikuto Kanno, Makoto Ouchi and Takaya Terashima*

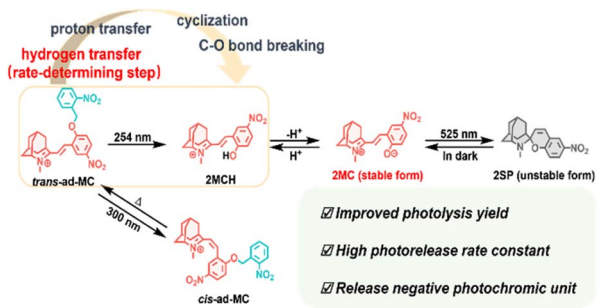
23111



Physically interpretable descriptors drive the materials design of metal hydrides for hydrogen storage

Seong-Hoon Jang,* Di Zhang, Hung Ba Tran, Xue Jia, Kiyoe Konno, Ryuhei Sato, Shin-ichi Orimo* and Hao Li*

23121



Tuning the photocaged spiropyran photoswitch with a sterically hindered adamantane group: releasing the stable merocyanine

Yifan Su, Xiang Li, Dexin Zheng, Joakim Andreásson, Hong Wang, Le Yu,* Jian Chen,* Jiani Ma* and Yu Fang

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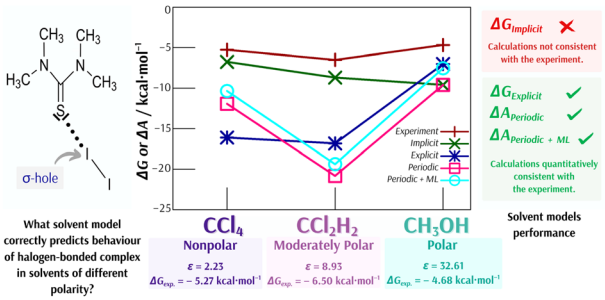
Solvation strategies for free-energy calculations in a halogen-bonded complex: implicit, explicit, and machine learning approaches

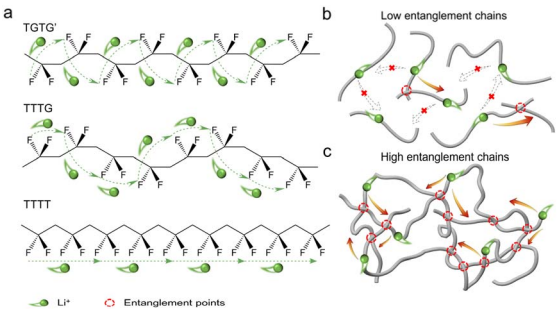
Jaroslav Vacek, Dávid Vrška, Debashree Manna,* Rabindranath Lo* and Pavel Hobza*



23139

Highly entangled P(VDF-TrFE) solid-state electrolytes for enhanced performance of solid-state lithium batteries

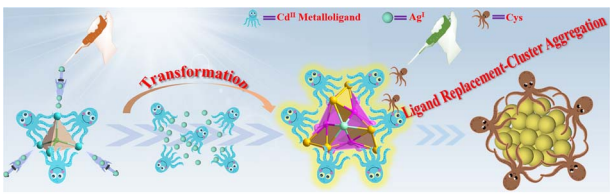
Hanghua Wu, Shuangfeng Li, Weiwei Zhu, Jie Zhang, Baohui Ren,* Yan-Fei Huang* and Zhong-Ming Li



23149

Light-induced access to a fluorescent Cd_7Ag_{21} nanocluster from a halide-supported Cd_8X nanocluster directed by a face-capping macrocyclic metalloligand

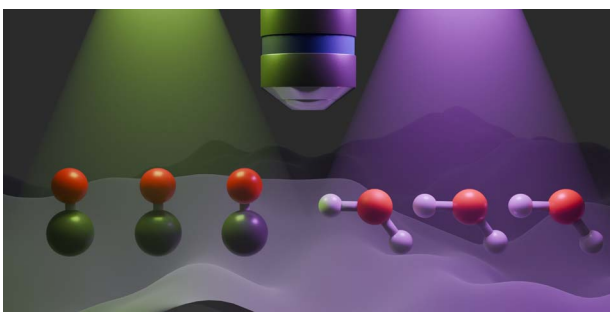
Biliu Lan, Ziling Li, Yanfang Feng, Tao Deng, Min Pan and Zhong Zhang*



23160

Mechanistic insights into the competition between electrochemical CO_2 reduction and hydrogen evolution on Ag-based electrocatalysts *via operando* Raman spectroscopy

Kinran Lau, Muhammad Adib Abdillah Mahbub, Nini Zhang, Anirudha Shekhawat, Xin Wang, Sabine Seisel, Ridha Zerdoumi and Wolfgang Schuhmann*



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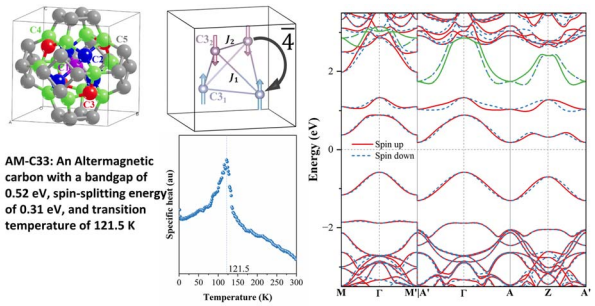
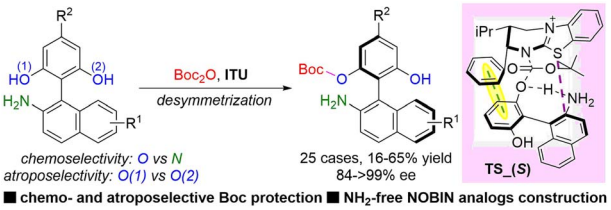


AM-C33: an altermagnetic carbon

Mingqing Liao,* Yuehua Wang, Pengcheng Ye, Chenggang Wu, Haoxin Jiang, Fei Zhou, Jintong Guan and Fengjiang Wang*

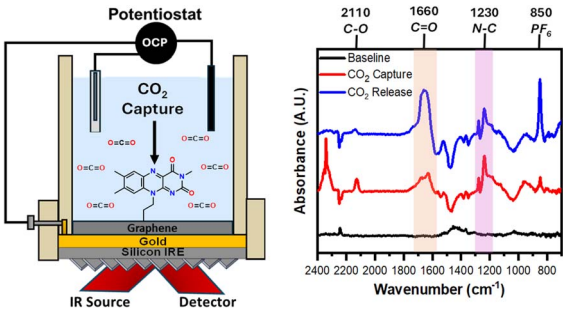
23181



Chemo- and atroposelective Boc protection for asymmetric synthesis of NH_2-free axially chiral biaryl amino phenols

Yangyang Wang, Yike Wang, Zhe Xu, Kexin Chen, Ying-guo Liu,* Xingkuan Chen,* Hongwei Zhou* and Jianfeng Xu*

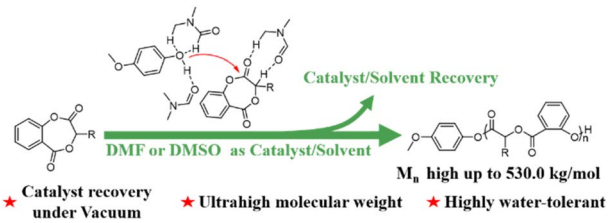
23189



Real-time monitoring of the reversible capture and release of CO_2 on anthraquinone and riboflavin-modified graphitic electrodes using ATR-SEIRAS

Abdur-Rahman Siddiqui, Joel Roberts, Jeanne N'Diaye, Alan L. Ferris, Kristin Martin, Seth T. Putnam, Rohit Bhargava, Jahan Dawlaty, Steven C. Zimmerman, Veronica Augustyn and Joaquín Rodríguez-López*

23203



DMF/DMSO-catalyzed selective ring-opening polymerization of salicylate cyclic esters

Ge Yao, Jiyu Liu, Hongjun Fu, Chunmei Wang, Guojie Li, Luya Cao, Xiaobo Pan and Jincai Wu*

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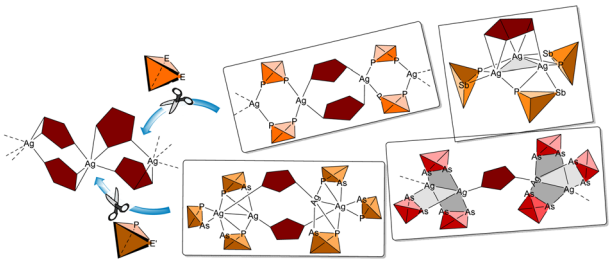
EDGE ARTICLES

23214

Two in one: a facile modular approach for the assembly of pnictogen-rich heteroleptic organometallic complexes

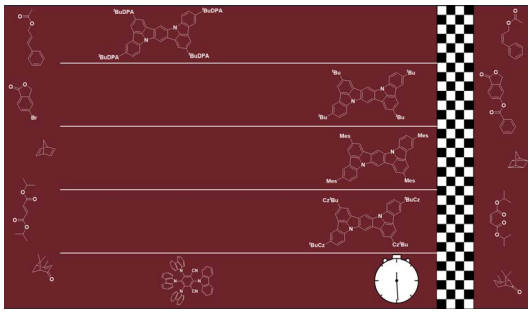
Bijan Mondal,* Christoph Riesinger and Manfred Scheer*



23220

DiICz MR-TADF emitters as potent energy transfer photocatalysts

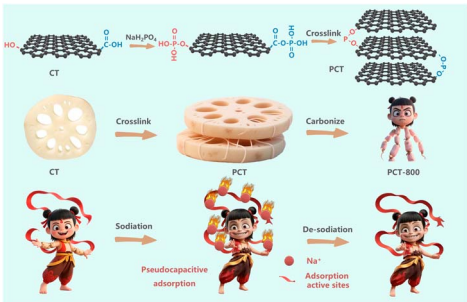
Lea Hämmerling, David Hall, Eliott Blin, Tabea Heil and Eli Zysman-Colman*



23233

Unraveling the origin of enhanced safety in capacitive-type carbon electrodes for 20C sodium-ion capacitors

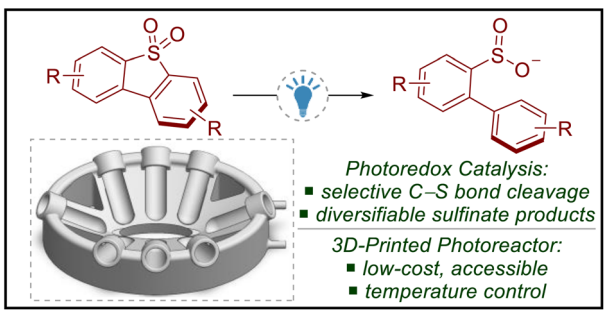
Bo Xiong, Jieming Cai, Biao Zhong, Luoming Zhang, Dongxiao Li, Jie Li, Juan Tian, Xiongwei Luo, Fei Yao, Zhiyu Zeng, Wentao Deng, Hongshuai Hou, Jialuo She,* Tianyun Qiu,* Guoqiang Zou,* Dulin Yin and Xiaobo Ji



23246

Photoredox catalysed reductive cleavage of dibenzothiophene dioxides enabled by a temperature-controlled photoreactor

Siyuan Wang, Quang Truong Le, Yoshiteru Shishido, Ismail Y. Kokculer, Ken Yamazaki, Gregory J. P. Perry,* Adrian M. Nightingale* and Hideki Yorimitsu*



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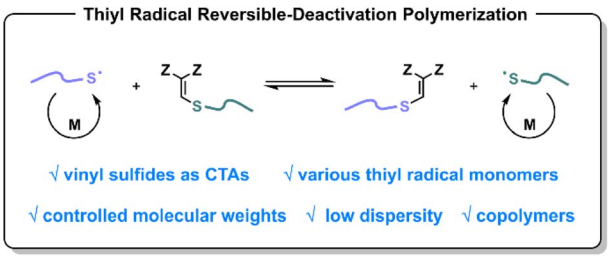
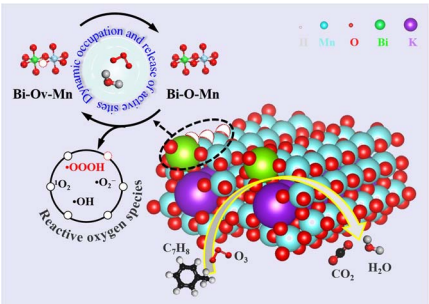
23253



Thiyl radical reversible-deactivation polymerization *via* degenerative transfer with vinyl sulfides

Huajuan Hu, Ping Yi, Derong Cao and Hanchu Huang*

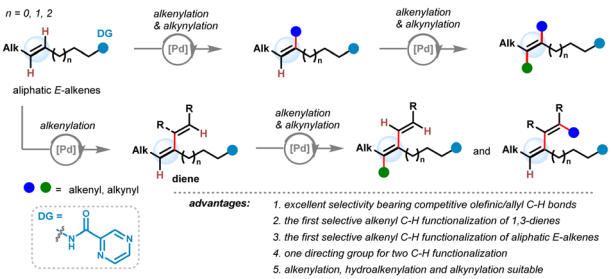
23262



Single site of water-resistant asymmetric Bi–Ov–Mn for robust VOC ozonation at ambient temperature

Yuqin Lu, Huayang Zhang, Hua Deng,* Jianguo Ding, Tingting Pan, Wenjie Tian, Yunbo Yu, Changbin Zhang, Wenpo Shan, Shaobin Wang, Hong He* and Joseph S. Francisco*

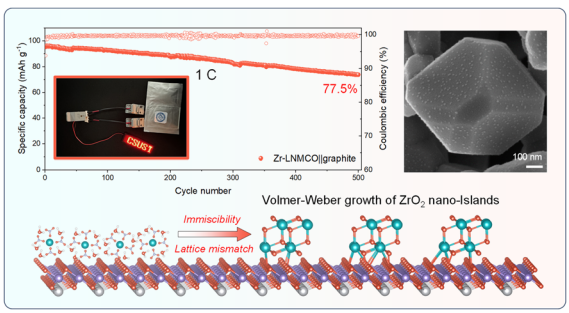
23271



Chelation-assisted multiple and relay C–H functionalization of unactivated aliphatic *E*-alkenes

Yini Wang, Xiaoli Li, Chengxing Peng, Yu Chen, Xi Lu, Yuhang Zhu, Peiyuan Yu,* Guofu Zhong* and Jian Zhang*

23282



Volmer–Weber growth of nano-island heterostructures on spinel cathodes: a route to stable high-voltage lithium-ion batteries

Gui Chu, Yuanqin She, Aoyu Huang, Qingquan Ye, Yimei Deng, Tongen Lin,* Yongqi Sun, Tobias U. Schülli,* Lianzhou Wang* and Xiaobo Zhu*

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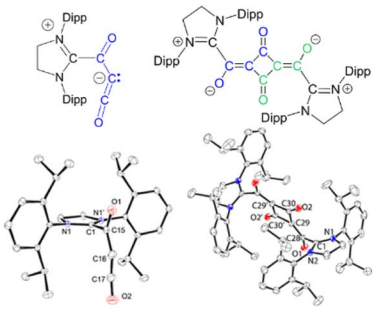
23292

Trapping carbon suboxide with a carbene and isolation of the carbene-stabilized carbon suboxide dimer

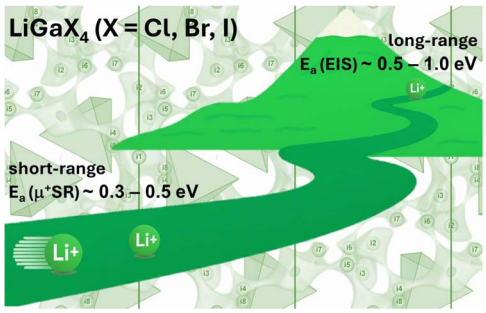
Tanner George, Erin R. Johnson and Jason D. Masuda*



23299

Insight into the prospects and limitations of mechanochemically-synthesised lithium tetrahalogallates, $LiGaX_4$ (X = Cl, Br, I), as Li-ion conductors

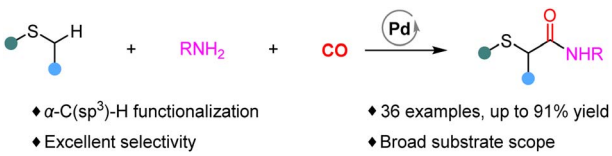
Nicolás Flores-González, Martí López, Nicolò Minafra, Jamie Jack, Jan Bohnenberger, Atsushi Inoishi, Nalin Gupta, Leandro Liborio, Francesc Viñes, Ronald I. Smith, Peter J. Baker, Ingo Krossing, Wolfgang G. Zeier, Francesc Illas and Duncan H. Gregory*



23310

Palladium-catalyzed amidocarbonylation of thioethers: access to α-amide-substituted thioether derivatives

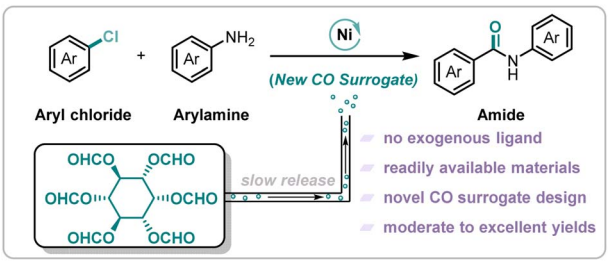
Xudong Mao, Le-Cheng Wang and Xiao-Feng Wu*



23315

Nickel-catalyzed aminocarbonylation of aryl chlorides enabled by a newly designed CO source

Zhen-Wei Liu, Yuanrui Wang, Ru-Han A. and Xiao-Feng Wu*



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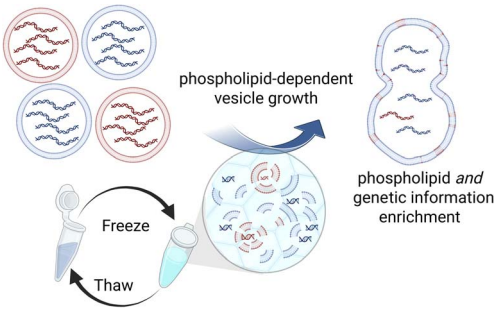
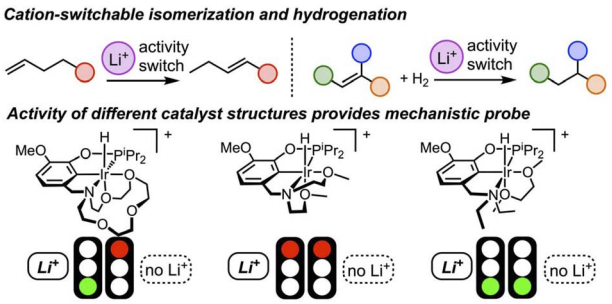
23321



Compositional selection of phospholipid compartments in icy environments drives the enrichment of encapsulated genetic information

Tatsuya Shinoda, Natsumi Noda, Takayoshi Watanabe, Kazumu Kaneko, Yasuhito Sekine and Tomoaki Matsuura*

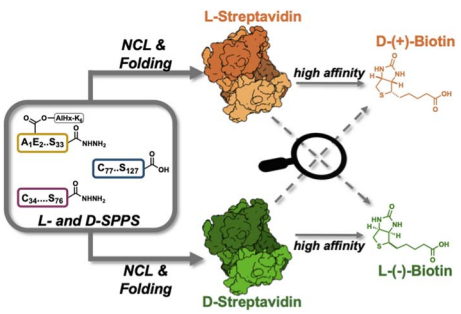
23330



Cation-switchable transposition and hydrogenation of alkenes *via* interconnected reaction mechanisms

Jonathan R. E. Cobb, Henry M. Dodge, Zoe E. Stuart, Elvis D. Perez Galarza, Shrabanti Bhattacharya, Changho Yoo, Chun-Hsing Chen and Alexander J. M. Miller*

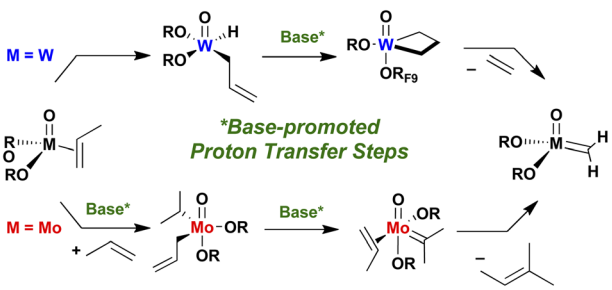
23342



Protein chirality as a determinant of ligand affinity: insights from L- and D-streptavidin

Riley J. Giesler, Peter C. S. Woodham, Steven R. E. Draper, Paul Spaltenstein, Frank G. Whitby, Christopher P. Hill and Michael S. Kay*

23351



Initiating olefin metathesis: alkylidenes from molecular Mo(IV)-oxo species, olefins and base-promoted proton transfer

Darryl F. Nater, Felix J. de Zwart, Nicolas Kaeffer and Christophe Copéret*

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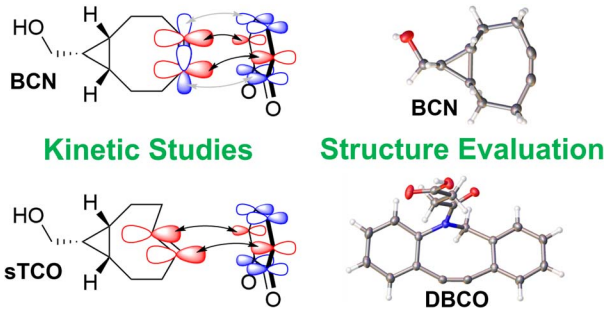
23357

Temperature–dependent reaction rates of quinone-alkene cycloaddition reveal that only entropy determines the rate of SPOCQ reactions

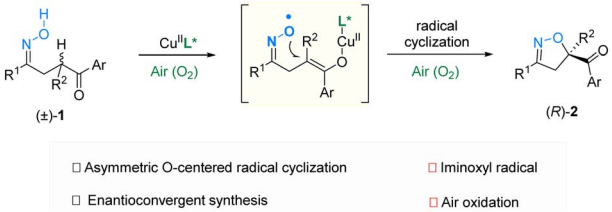
Johannes A. M. Damen, Jorge Escorihuela, Judith Firet, Han Zuilhof* and Bauke Albada*



23366

Cu-catalyzed enantioconvergent oxygen-centered radical cyclization

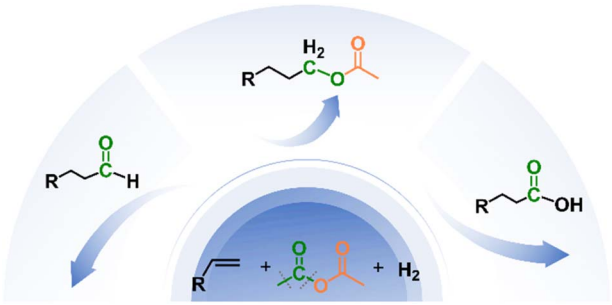
Zhen-Yu Li, Chun-Dong Huang, Chun-Yan Guan, Hui-Min Guo, Ling-Min Liu, Xiao Xiao, Beiling Gao,* Shao-Fei Ni* and Guang-Jian Mei*



23376

Acetic anhydride as a versatile carbon source in carbonylation reactions

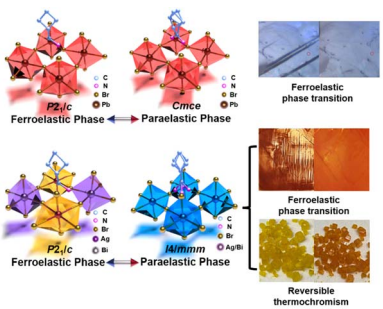
Yanru Zhang, Ying Wang,* Junfeng Xiang, Yanyan Wang, Longbo Zhang, Jun He, Chenglong Yu, Jia Guo, Jie Cui, Xing Tong, Ziwei Zhao, Tianbin Wu, Qingli Qian* and Buxing Han*



23385

Two-dimensional lead-free double perovskite ferroelastics with dynamic thermochromism

Chang-Yuan Su,* Heng-Guan Yi, Hao-Fei Ni, Guo-Wei Du, San-Qiang Xia, Zunqi Liu,* Zhi-Xu Zhang* and Da-Wei Fu*



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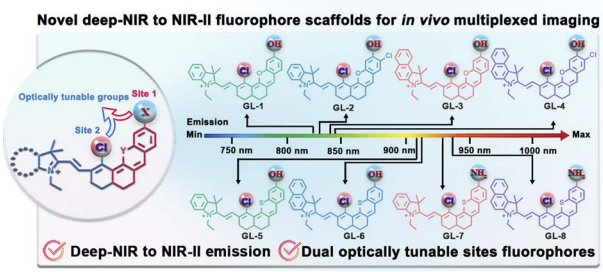
23394



Deep-NIR to NIR-II hemicyanine fluorophore scaffolds with dual optically tunable sites for *in vivo* multiplexed imaging

Qinian Liu, Zhuoyang Li, Yujie Huang, Zhenni Lin, Xing-Can Shen* and Hua Chen*

CORRECTIONS

23405

Correction: Capturing and labeling CO_2 in a jar: mechanochemical ^{17}O-enrichment and ssNMR study of sodium and potassium (bi)carbonate salts

Austin Peach,* Nicolas Fabregue, Célia Erre, Thomas-Xavier Métro, David Gajan, Frédéric Mentink-Vigier, Faith Scott, Julien Trébosc, Florian Voron, Nicolas Patris, Christel Gervais and Danielle Laurencin*

23408

Correction: Structural insights into a bacterial terpene cyclase fused with haloacid dehalogenase-like phosphatase

Keisuke Fujiyama, Hiroshi Takagi, Nhu Ngoc Quynh Vo, Naoko Morita, Toshihiko Nogawa and Shunji Takahashi*

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