

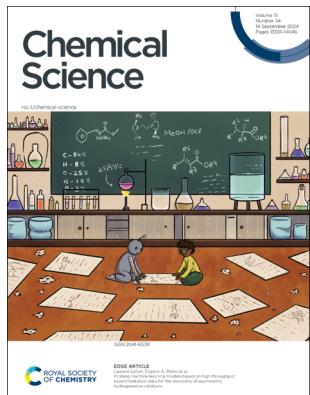
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ISSN 2041-6539 CODEN CSHCBM 15(34) 13561–14046 (2024)



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See Laurent Lefort, Evgeny A. Pidko *et al.*, pp. 13618–13630. Image reproduced by permission of Evgeny A. Pidko from *Chem. Sci.*, 2024, 15, 13618.



Inside cover

See Alexander Lemmens, Musahid Ahmed *et al.*, pp. 13631–13637. Image reproduced by permission of Mieke Dericx, Triet Dang and Alexander Lemmens from *Chem. Sci.*, 2024, 15, 13631.

REVIEWS

13576

The efficient synthesis of three-membered rings via photo- and electrochemical strategies

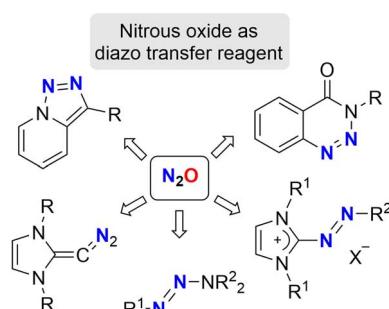
Xinyu Han, Na Zhang, Qiannan Li, Yu Zhang* and Shoubhik Das*



13605

Nitrous oxide as diazo transfer reagent

Alexandre Genoux and Kay Severin*



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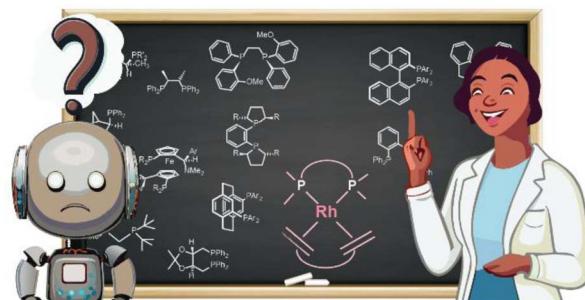
Fundamental questions
Elemental answers

EDGE ARTICLES

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Probing machine learning models based on high throughput experimentation data for the discovery of asymmetric hydrogenation catalysts

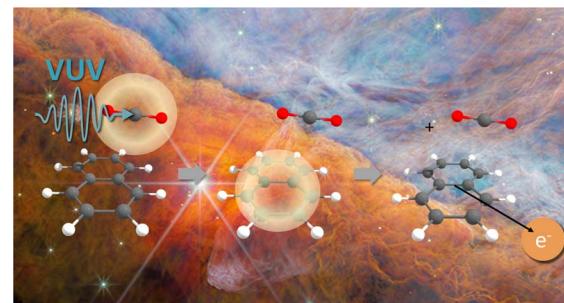
Adarsh V. Kalikadien, Cecile Valsecchi, Robbert van Putten, Tor Maes, Mikko Muuronen, Natalia Dyubankova, Laurent Lefort* and Evgeny A. Pidko*



13631

Electronic energy transfer ionization in naphthalene–CO₂ clusters reveals excited states of dry ice

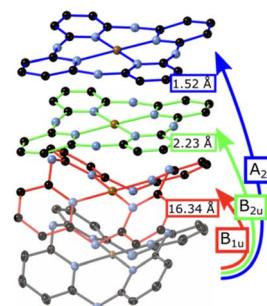
Alexander K. Lemmens, Anna Wannenmacher, Nureshan Dias and Musahid Ahmed*



13638

Quantifying near-symmetric molecular distortion using symmetry-coordinate structural decomposition

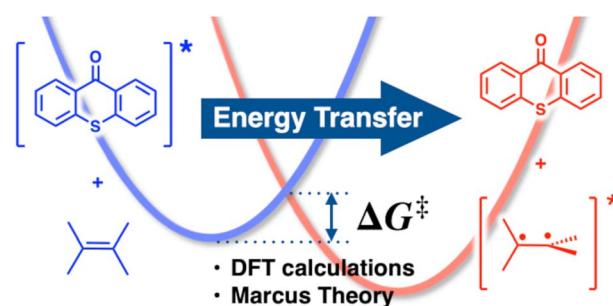
Christopher J. Kingsbury* and Mathias O. Senge*



13650

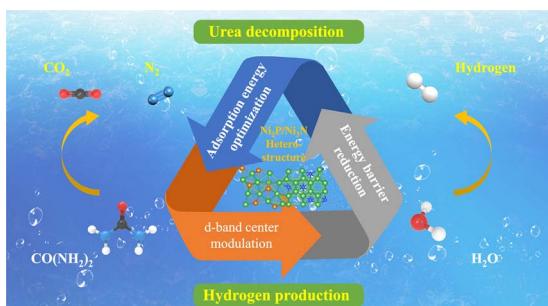
Straightforward computational determination of energy-transfer kinetics through the application of the Marcus theory

Albert Solé-Daura and Feliu Maseras*



EDGE ARTICLES

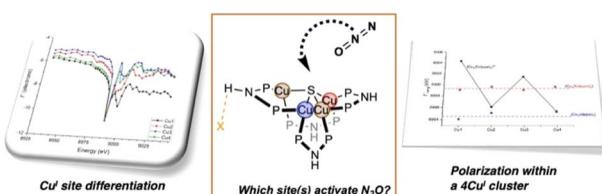
13659



Built-in electrophilic/nucleophilic domain of nitrogen-doped carbon nanofiber-confined Ni₂P/Ni₃N nanoparticles for efficient urea-containing water-splitting reactions

Jiaxin Li, Chun Yin, Shuli Wang, Baogang Zhang* and Ligang Feng*

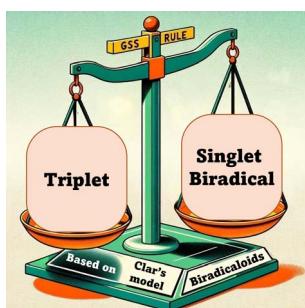
13668



Cu site differentiation in tetracopper(I) sulfide clusters enables biomimetic N₂O reduction

Pinar Alayoglu, Suresh C. Rathnayaka, Tieyan Chang, SuYin Grass Wang, Yu-Sheng Chen and Neal P. Mankad*

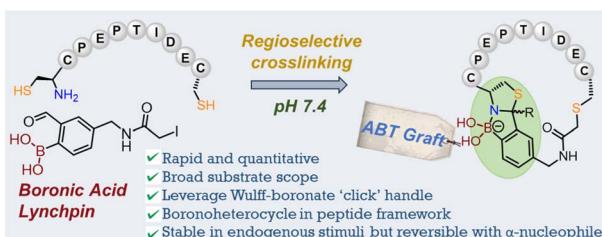
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Prediction of the ground state for indenofluorene-type systems with Clar's π -sextet model

Gibu George, Anton J. Stasyuk* and Miquel Solà*

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Harnessing a bis-electrophilic boronic acid lynchpin for azaborolo thiazolidine (ABT) grafting in cyclic peptides

Basab Kanti Das, Arnab Chowdhury, Saurav Chatterjee, Nitesh Mani Tripathi, Bibekananda Pati, Soumit Dutta and Anupam Bandyopadhyay*

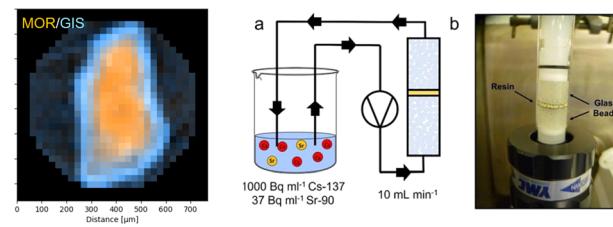


EDGE ARTICLES

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Engineered species-selective ion-exchange in tuneable dual-phase zeolite composites

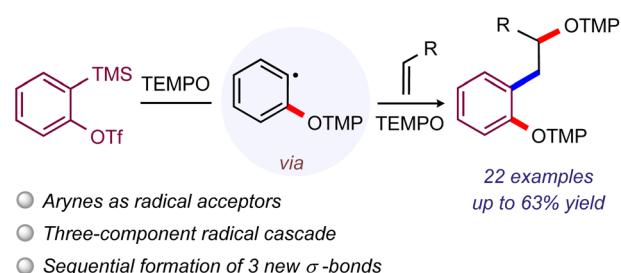
James L. A. Reed, Andrew James, Thomas Carey, Neelam Fitzgerald, Simon Kellet, Antony Nearchou, Adele L. Farrelly, Harrison A. H. Fell, Phoebe K. Allan* and Joseph A. Hriljac*



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Intermolecular radical oxyalkylation of arynes with alkenes and TEMPO

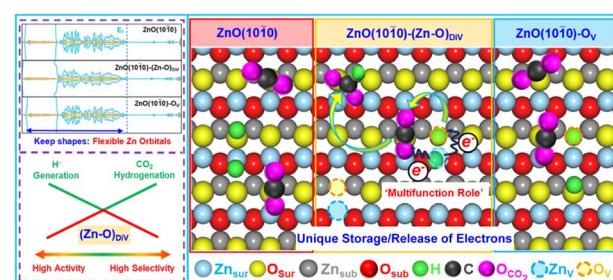
Debkanta Bhattacharya, Maximilian Scherübl, Constantin G. Daniliuc and Armido Studer*



13717

Theoretical insights into the generation and reactivity of hydride on the ZnO(1010) surface

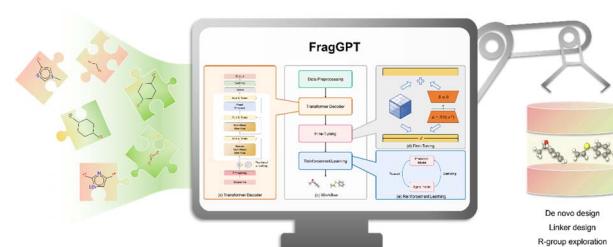
Xian-Yang Zhang, Zhi-Qiang Wang* and Xue-Qing Gong*



13727

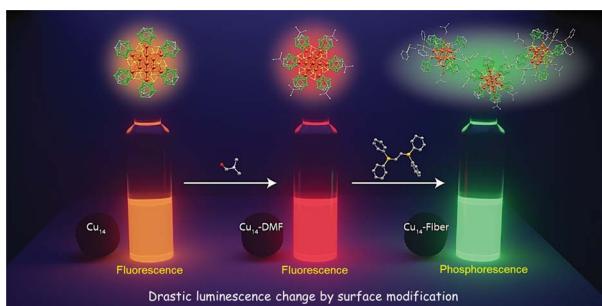
Unlocking comprehensive molecular design across all scenarios with large language model and unordered chemical language

Jie Yue, Bingxin Peng, Yu Chen, Jieyu Jin, Xinda Zhao, Chao Shen, Xiangyang Ji, Chang-Yu Hsieh, Jianfei Song,* Tingjun Hou,* Yafeng Deng* and Jike Wang*



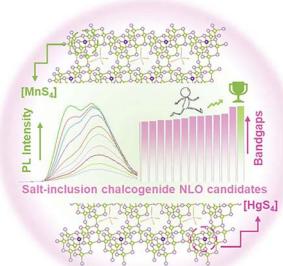
EDGE ARTICLES

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**Multicolor photoluminescence of Cu₁₄ clusters modulated using surface ligands**

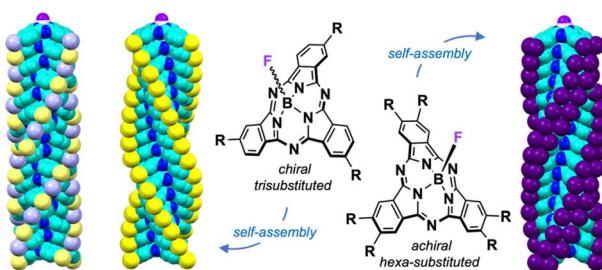
Arijit Jana, Subrata Duary, Amitabha Das, Amoghavarsha Ramachandra Kini, Swetashree Acharya, Jan Machacek, Biswarup Pathak,* Tomas Base* and Thalappil Pradeep*

13753

**Salt-inclusion chalcogenides with d-orbital components: unveiling remarkable nonlinear optical properties and dual-band photoluminescence**

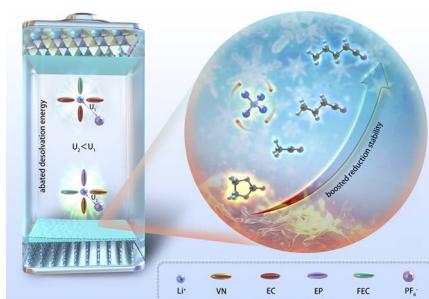
Shao-Min Pei, Ming-Shu Zhang, Fan Wu, Yan Guo, Xiao-Ming Jiang, Bin-Wen Liu* and Guo-Cong Guo*

13760

**The key role of chirality and peripheral substitution in the columnar organization of bowl-shaped subphthalocyanines**

Jorge Labella,* Elisa López-Serrano, Daniel Aranda, María J. Mayoral, Enrique Ortí* and Tomás Torres*

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**A nitrile solvent structure induced stable solid electrolyte interphase for wide-temperature lithium-ion batteries**

Zhongming Wang, Zhiyuan He, Zhongsheng Wang, Jixu Yang, Kecheng Long, Zhibin Wu, Gang Zhou, Lin Mei* and Libao Chen*

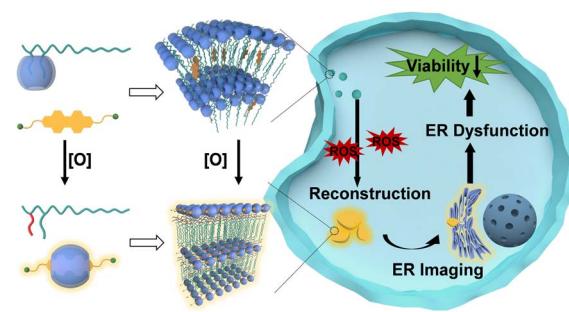


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Host–guest binding between cucurbit[8]uril and amphiphilic peptides achieved tunable supramolecular aggregates for cancer diagnosis

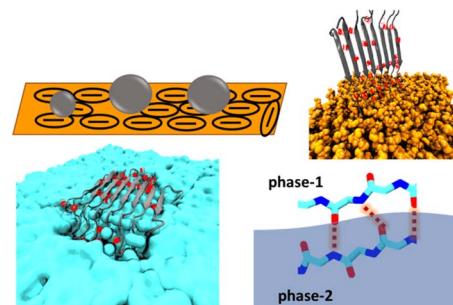
Jie Niu, Jie Yu, Xuan Wu, Ying-Ming Zhang,* Yong Chen, ZhiLin Yu and Yu Liu*



13788

The molecular basis for the increased stability of the FUS-LC fibril at the anionic membrane- and air–water interfaces

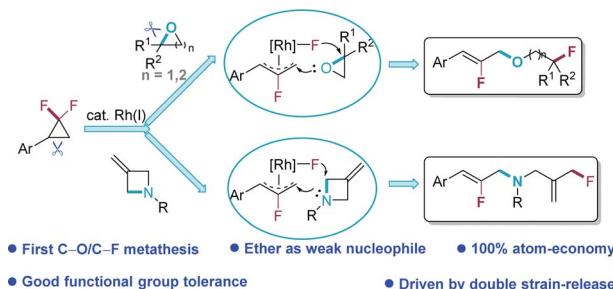
Sanjoy Paul, Sayantan Mondal, Irina Shenogina and Qiang Cui*



13800

Double strain-release enables formal C–O/C–F and C–N/C–F ring-opening metathesis

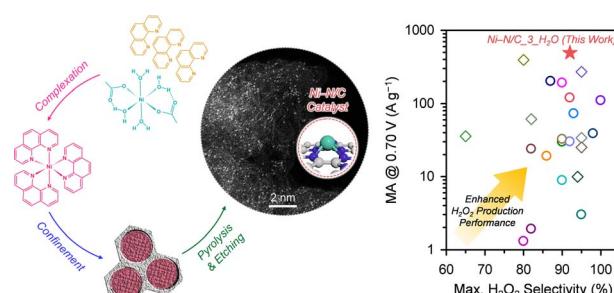
Yulei Zhu, Jie Jia, Xiangyu Song, Chunyu Gong* and Ying Xia*



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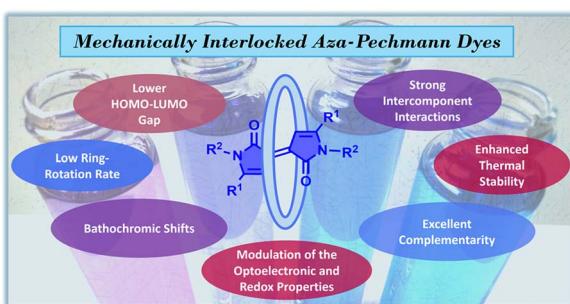
Understanding the preparative chemistry of atomically dispersed nickel catalysts for achieving high-efficiency H₂O₂ electrosynthesis

June Sung Lim, Jinwoo Woo, Geunsu Bae, Suhwan Yoo, Jinjong Kim, Jae Hyung Kim, Jong Hoon Lee, Young Jin Sa, Ji-Wook Jang, Yun Jeong Hwang, Chang Hyuck Choi* and Sang Hoon Joo*



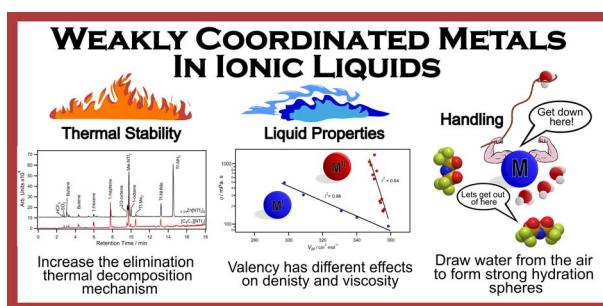
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**Mechanical insulation of aza-Pechmann dyes within [2]rotaxanes**

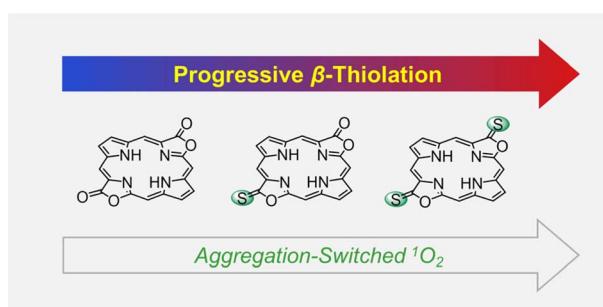
Guillermo Cutillas-Font, Aurelia Pastor,* Mateo Alajarín, Alberto Martínez-Cuevav, Marta Marín-Luna, Belén Batanero and José Berna*

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**A thermophysical investigation of weakly coordinated metals in ionic liquids**

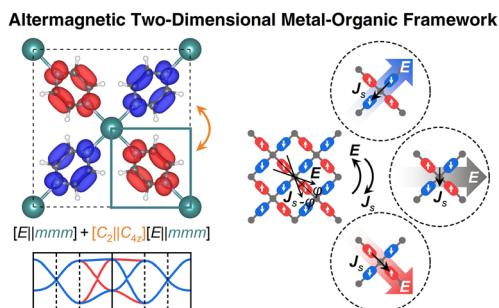
Coby J. Clarke,* Thomas Clayton, Matthew J. Palmer, Kevin R. J. Lovelock and Peter Licence

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**More is different: progressive β -thiolation induced-porphyrin aggregation switches singlet oxygen photosensitization**

Mengliang Zhu, Hang Zhang, Yuhang Yao, Mingpu Wen, Guangliu Ran, Yi Yu, Ruijing Zhang, Xing-Jie Liang, Jing Zhang, Wenkai Zhang* and Jun-Long Zhang*

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**Realizing altermagnetism in two-dimensional metal–organic framework semiconductors with electric-field-controlled anisotropic spin current**

Yixuan Che, Haifeng Lv,* Xiaojun Wu* and Jinlong Yang

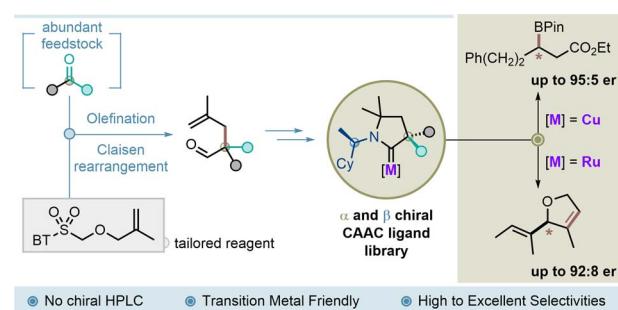


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Streamlined synthetic assembly of α -chiral CAAC ligands and catalytic performance of their copper and ruthenium complexes

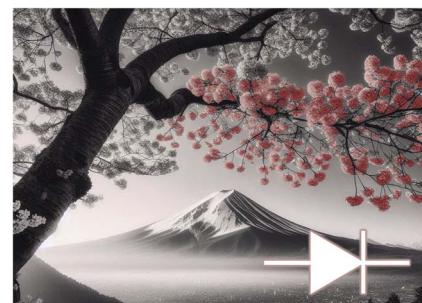
Adrien Madron du Vigné and Nicolai Cramer*



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Catalytic resonance theory: the catalytic mechanics of programmable ratchets

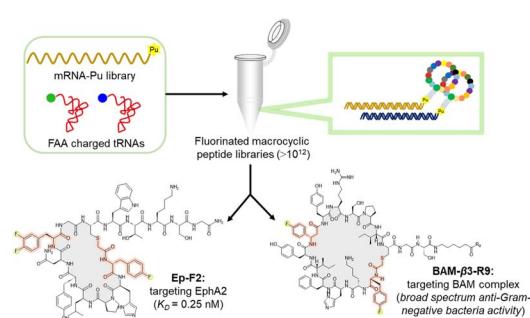
Madeline A. Murphy, Sallye R. Gathmann, Rachel Getman, Lars Grabow, Omar A. Abdelrahman and Paul J. Dauenhauer*



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Ribosomal translation of fluorinated non-canonical amino acids for *de novo* biologically active fluorinated macrocyclic peptides

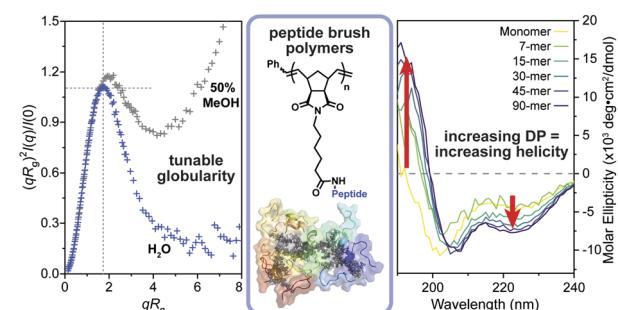
Junjie Wu, Yuchan Wang, Wenfeng Cai, Danyan Chen, Xiangda Peng, Huilei Dong, Jinjing Li, Hongtan Liu, Shuting Shi, Sen Tang, Zhifeng Li, Haiyan Sui, Yan Wang, Chuanliu Wu, Youming Zhang,* Xinmiao Fu* and Yizhen Yin*



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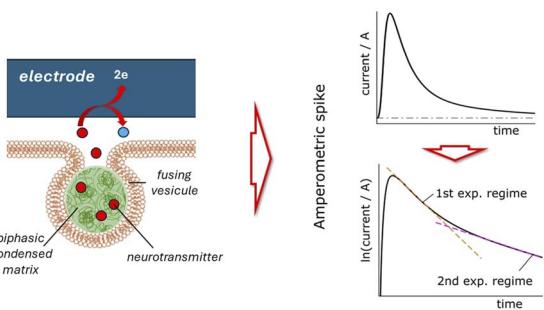
Conformational modulation and polymerization-induced folding of proteomimetic peptide brush polymers

Julia Oktawiec, Omar M. Ebrahim, Yu Chen, Kaylen Su, Christopher Sharpe, Nathan D. Rosenmann, Clara Barbut, Steven J. Weigand, Matthew P. Thompson, James Byrnes, Baofu Qiao and Nathan C. Gianneschi*



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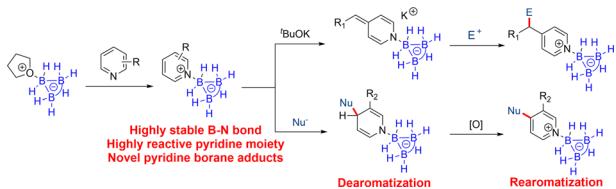
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Vesicular neurotransmitters exocytosis monitored by amperometry: theoretical quantitative links between experimental current spikes shapes and intravesicular structures

Reina Dannaoui, Ren Hu, Lihui Hu, Zhong-Qun Tian, Irina Svir, Wei-Hua Huang, Christian Amatore* and Alexander Oleinick*

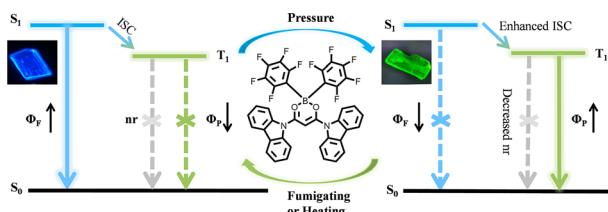
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Triborane (B_3H_7)-mediated regioselective substitution reactions of pyridine derivatives

Zi-Heng Fan, Jia-Xin Kang, Sihan Jia, Qiao-Jing Pan, Lei Cao, Xi-Meng Chen, Cong-Qiao Xu, Yan-Na Ma* and Xuenian Chen*

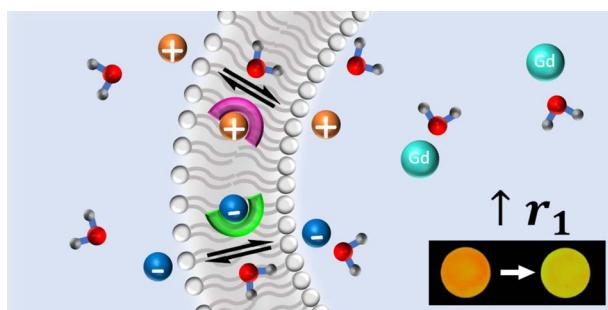
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Reversible switching from fluorescence to room temperature phosphorescence amplified by exciton-vibration coupling through pressure-induced tiny packing changes

Yangyang Cao, Zhenzhen Xu,* Xinyuqi Zhao, Yong Yang, Haoran Liu, Pingyang Wang, Miao Yu, Hao Li and Hongbing Fu*

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Ion carrier modulated MRI contrast

Anna M. Duncan, Connor M. Ellis, Hannah Livingston, Aidan Kerckhoff, Ferenc E. Mózes, Matthew J. Langton and Jason J. Davis*

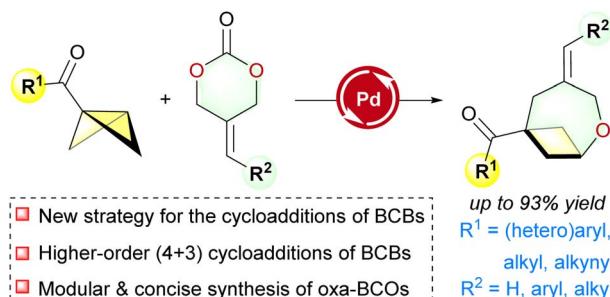


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Palladium-catalyzed decarboxylative (4 + 3) cycloadditions of bicyclobutanes with 2-alkylidenetrimethylene carbonates for the synthesis of 2-oxabicyclo[4.1.1]octanes

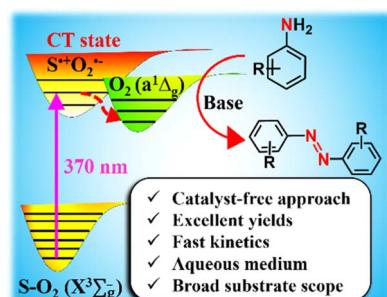
Xin-Yu Gao, Lei Tang, Xu Zhang and Jian-Jun Feng*



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Photosensitizer-free singlet oxygen generation via a charge transfer transition involving molecular O₂ toward highly efficient oxidative coupling of arylamines to azoaromatics

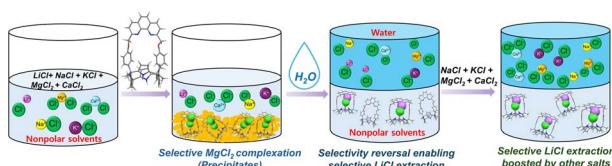
Shivendra Singh and Tushar Kanti Mukherjee*



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Ion pair extractant selective for LiCl and LiBr

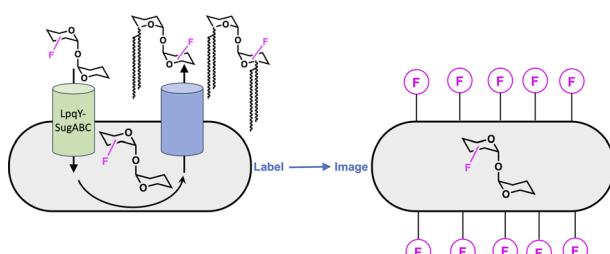
Nam Jung Heo, Ju Hyun Oh, Aimin Li, Kyoungsoon Lee, Qing He, Jonathan L. Sessler* and Sung Kuk Kim*



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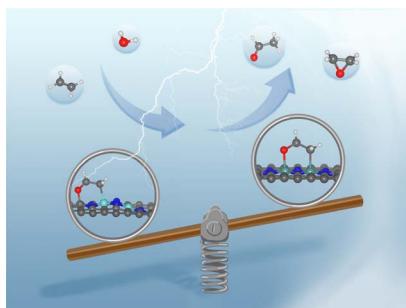
Fluorinated trehalose analogues for cell surface engineering and imaging of *Mycobacterium tuberculosis*

Collette S. Guy, James A. Gott, Jonathan Ramírez-Cárdenas, Christopher de Wolf, Christopher M. Furze, Geoff West, Juan C. Muñoz-García, Jesus Angulo and Elizabeth Fullam*



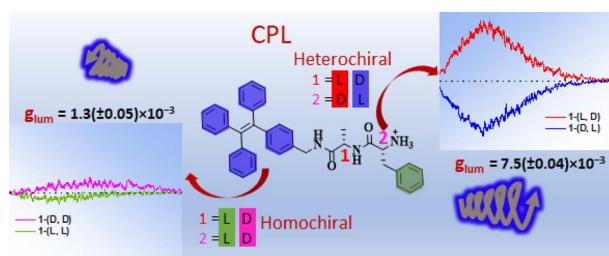
EDGE ARTICLES

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Carbon–metal versus metal–metal synergistic mechanism of ethylene electro-oxidation *via* electrolysis of water on TM₂N₆ sites in graphene

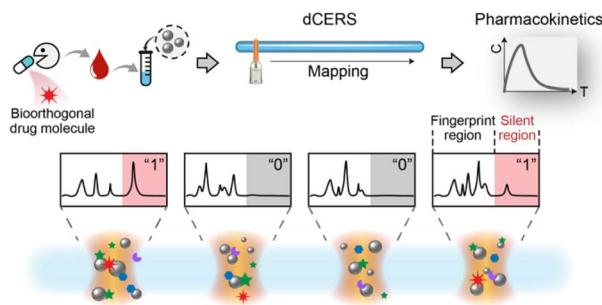
 Yun-Jie Chu, Chang-Yan Zhu, Chun-Guang Liu,*
 Yun Geng, Zhong-Min Su and Min Zhang*

13987


Enhanced circularly polarized luminescence attained *via* self-assembly of heterochiral as opposed to homochiral dipeptides in water

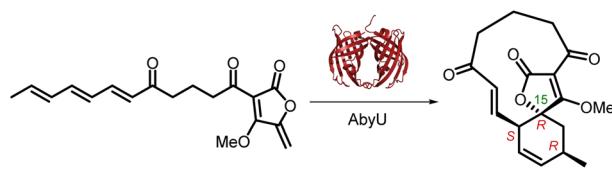
Sayan Bera, Umesh and Santanu Bhattacharya*

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Digital colloid-enhanced Raman spectroscopy for the pharmacokinetic detection of bioorthogonal drugs

Xinyuan Bi, Zhicheng He, Zhewen Luo, Wensi Huang, Xingxing Diao and Jian Ye*

14009


Antibiotic origami: selective formation of spirotetroneates in abyssomicin biosynthesis

Sbusisiwe Z. Mbatha, Catherine R. Back, Andrew J. Devine, Hannah M. Mulliner, Samuel T. Johns, Harry Lewin, Kaiman A. Cheung, Katja Zorn, James E. M. Stach, Martin A. Hayes, Marc W. van der Kamp, Paul R. Race* and Christine L. Willis*

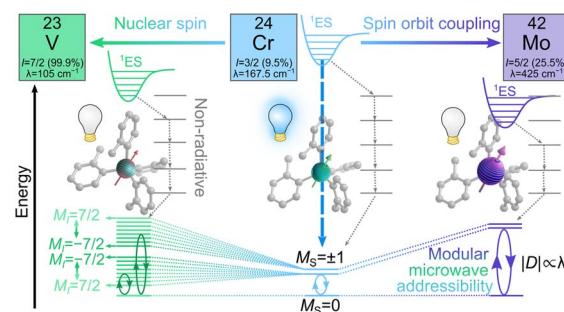


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14016

Coherent spin-control of $S = 1$ vanadium and molybdenum complexes

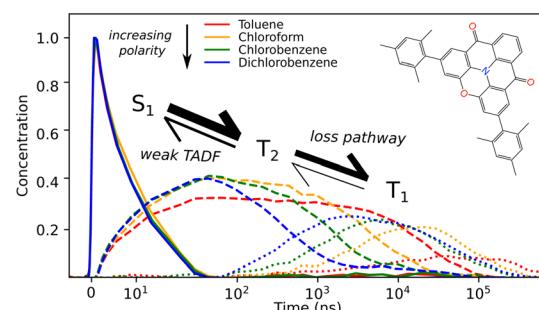
Daniel W. Laorenza, Kathleen R. Mullin, Leah R. Weiss,
Sam L. Bayliss, Pratiti Deb, David D. Awschalom,*
James M. Rondinelli* and Danna E. Freedman*



14027

Triplet dynamics reveal loss pathways in multi-resonance thermally activated delayed fluorescence emitters

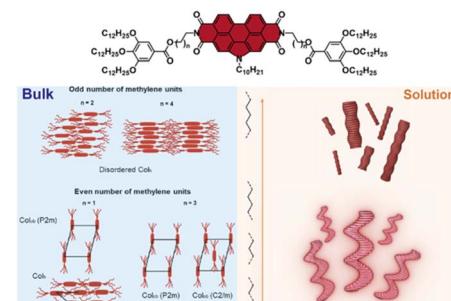
Alexandra N. Stuart,* Katrina Bergmann, Inseong Cho,
William J. Kendrick, Zachary M. Hudson,
Wallace W. H. Wong and Girish Lakhwani*



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Supramolecular polymerization and bulk properties relationship in ester-functionalized *N*-annulated perylenediimides

Lucía López-Gandul, Giulia Lavarda, Bart W. L. van den Bersselaar, Ghislaine Vantomme, E. W. Meijer*
and Luis Sánchez*



CORRECTION

14044

Correction: Real-time structural dynamics of the ultrafast solvation process around photo-excited aqueous halides

Verena Markmann,* Jaysree Pan, Bianca L. Hansen, Morten L. Haubro, Amke Nimmrich, Philipp Lenzen,
Matteo Levantino, Tetsuo Katayama, Shin-ichi Adachi, Simone Gorski-Bilke, Friedrich Temps, Asmus O. Dohn, Klaus
B. Møller, Martin M. Nielsen and Kristoffer Haldrup

