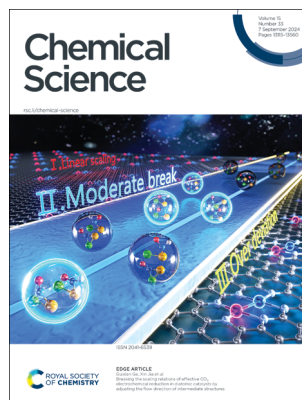


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ISSN 2041-6539 CODEN CSHCBM 15(33) 13115–13560 (2024)



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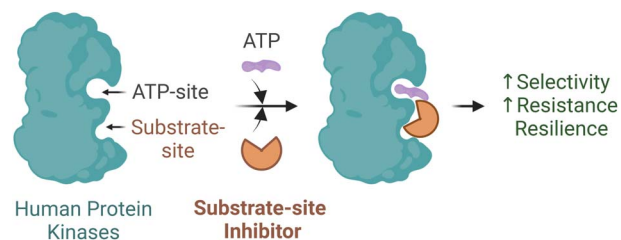
Inside cover
See Guixian Ge, Xin Jia *et al.*, pp. 13160–13172. Image reproduced by permission of Xin Jia from *Chem. Sci.*, 2024, 15, 13160.

REVIEW

13130

The prospect of substrate-based kinase inhibitors to improve target selectivity and overcome drug resistance

Biswajit Biswas, Yen-Hua Huang, David J. Craik* and Conan K. Wang*

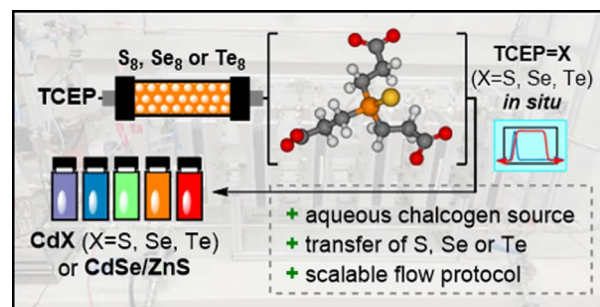


EDGE ARTICLES

13148

An innovative chalcogenide transfer agent for improved aqueous quantum dot synthesis

Guillaume Petit, Cedric Malherbe, Pauline Bianchi and Jean-Christophe M. Monbaliu*



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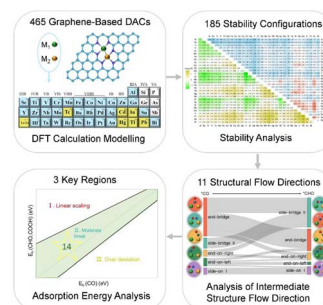
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13160

Breaking the scaling relations of effective CO₂ electrochemical reduction in diatomic catalysts by adjusting the flow direction of intermediate structures

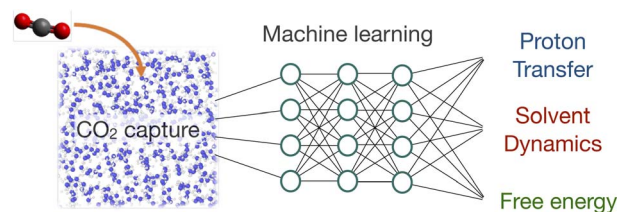
Yanwen Zhang, Zhaoqun Yao, YiMing Yang, Xingwu Zhai, Feng Zhang, Zhirong Guo, Xinghuan Liu, Bin Yang, Yunxia Liang, Guixian Ge* and Xin Jia*



13173

Machine learning demonstrates the impact of proton transfer and solvent dynamics on CO₂ capture in liquid ammonia

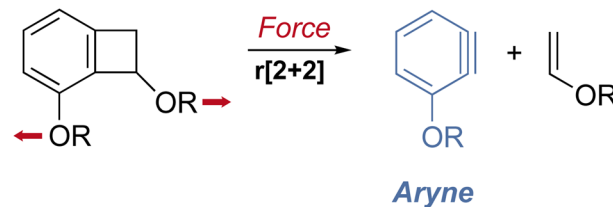
Marcos F. Calegari Andrade,* Sichi Li,* Tuan Anh Pham, Sneha A. Akhade and Simon H. Pang*



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Mechanochemical generation of aryne

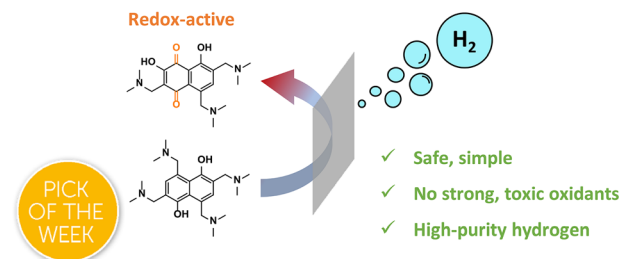
Qianqian Cheng and Guillaume De Bo*



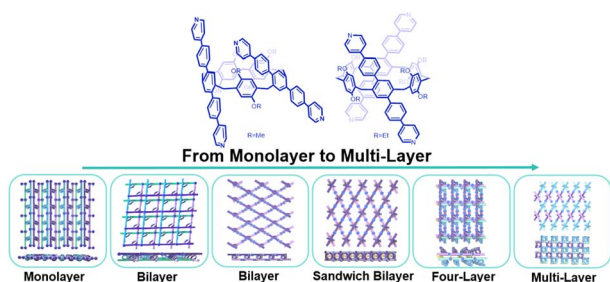
13185

In situ electrosynthesis of quinone-based redox-active molecules coupling with high-purity hydrogen production

Hyunjoon Ji, Ziming Zhao, Changkun Zhang* and Xianfeng Li*



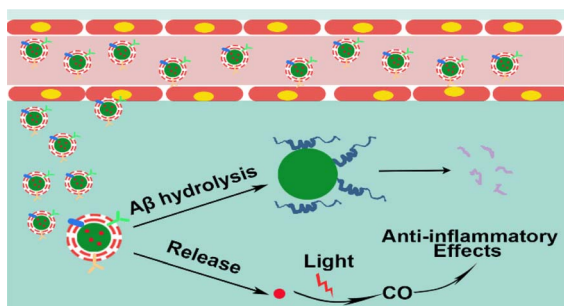
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Accurate construction of monolayer, bilayer, sandwich bilayer, four-layer, multi-layer and chiral bilayer 2D pillararene-type supramolecular networks

Zhao-Nian Chen, Le-Ping Zhang, Huai-Li Wu, Qiao-Yan Qi, Meng Yan, Jia Tian, Guan-Yu Yang, Zhan-Ting Li* and Bo Yang*

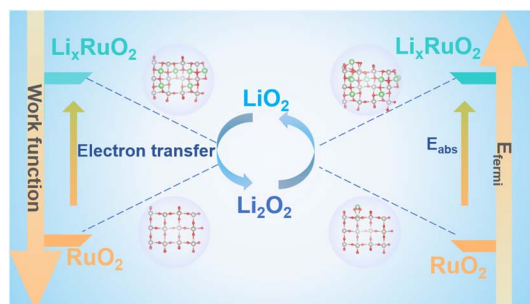
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Biomimetic engineering of a neuroinflammation-targeted MOF nanozyme scaffolded with photo-trigger released CO for the treatment of Alzheimer's disease

Chun Liu, Wenting Zhang, Haochen Zhang, Chuanqi Zhao, Xiubo Du, Jinsong Ren and Xiaogang Qu*

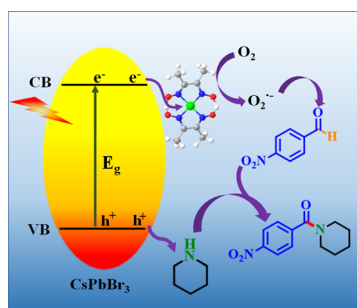
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Unleashing the potential of Li-O₂ batteries with electronic modulation and lattice strain in pre-lithiated electrocatalysts

Zhengcai Zhang, Dulin Huang, Shuochao Xing, Minghui Li, Jing Wu, Zhang Zhang, Yaying Dou* and Zhen Zhou*

13218



Deciphering charge transfer dynamics of a lead halide perovskite-nickel(II) complex for visible light photoredox C-N coupling

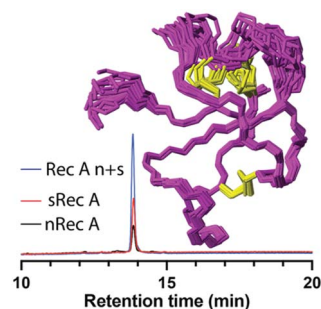
Vishesh Kumar, Sunil Kumar Patel, Ved Vyas, Deepak Kumar, E. Siva Subramaniam Iyer* and Arindam Indra*



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Picking the tyrosine-lock: chemical synthesis of the tyrosyl-DNA phosphodiesterase I inhibitor recifin A and analogues

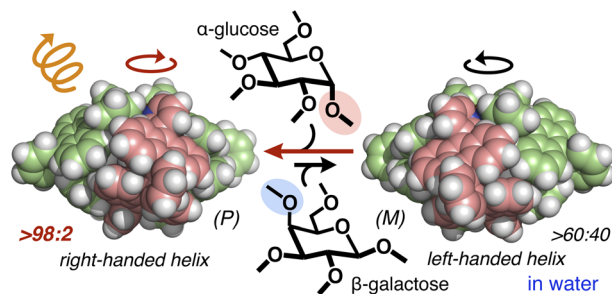
Taylor B. Smallwood, Lauren R. H. Krumpke, Colton D. Payne, Victoria G. Klein, Barry R. O'Keefe, Richard J. Clark,* Christina I. Schroeder* and K. Johan Rosengren*



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Helicity control of a polyaromatic coordination capsule through stereoselective CH- π interactions

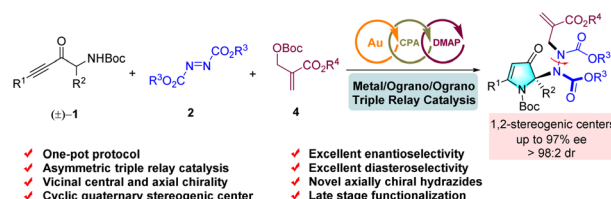
Natsuki Kishida, Hayate Sasafuchi, Tomohisa Sawada and Michito Yoshizawa*



13240

Enantioconvergent and diastereoselective synthesis of atropisomeric hydrazides bearing a cyclic quaternary stereocenter through ternary catalysis

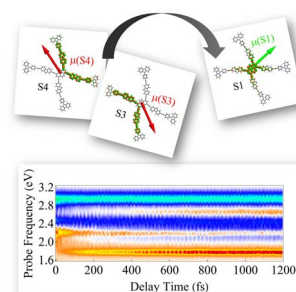
Xia Wang, Shao-Jie Wang, Xiaolan Xin, Hao An, Zhifeng Tu,* Hui Yang, Ming Wah Wong* and Shenci Lu*



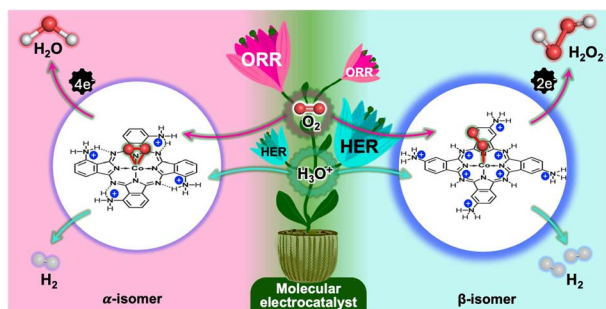
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Transient-absorption spectroscopy of dendrimers via nonadiabatic excited-state dynamics simulations

Royle Perez-Castillo, Victor M. Freixas, Shaul Mukamel, Aliezer Martinez-Mesa, Llinersy Uranga-Piña, Sergei Tretiak, Maxim F. Gelin and Sebastian Fernandez-Alberti*



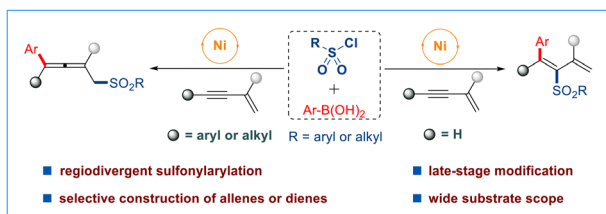
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Switchable molecular electrocatalysis

Shifali Dutt, Alagar Raja Kottaichamy, Neethu Christudas Dargily, Sanchayita Mukhopadhyay, Bhojkumar Nayak, Mruthyunjayachari Chattanhali Devendrachari, Chatakudhath Prabakaran Vinod, Harish Makri Nimbegondi Kotresh and Musthafa Ottakam Thotiyl*

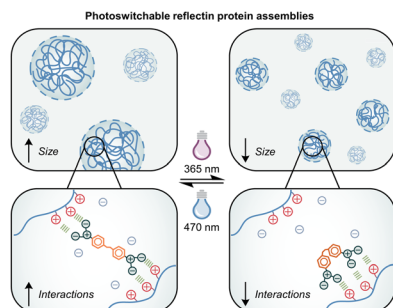
13271



Nickel-catalyzed regiodivergent sulfonylarylation of 1,3-enynes to access allenes and dienes

Zhuomin Chi, Yongchao Zhou, Bingbing Liu, Xiaojing Xu, Xueyuan Liu and Yongmin Liang*

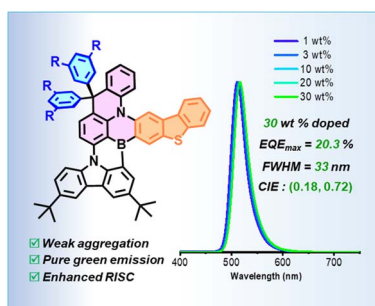
13279



Reversible and size-controlled assembly of reflectin proteins using a charged azobenzene photoswitch

Cassidy M. Tobin, Reid Gordon, Seren K. Tochikura, Bradley F. Chmelka, Daniel E. Morse and Javier Read de Alaniz*

13290



10-Dibenzothiophenyl-9,9-diphenylacridane-based multiple resonance emitters for high-efficiency narrowband green OLEDs with CIE $y > 0.7$ at high doping concentrations

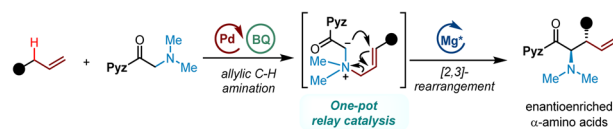
Rui Zhong, Mengyu Wang, Xingdong Wang, Shumeng Wang, Shiyang Shao* and Lixiang Wang*



13299

Tandem catalytic allylic C–H amination and asymmetric [2,3]-rearrangement *via* bimetallic relay catalysis

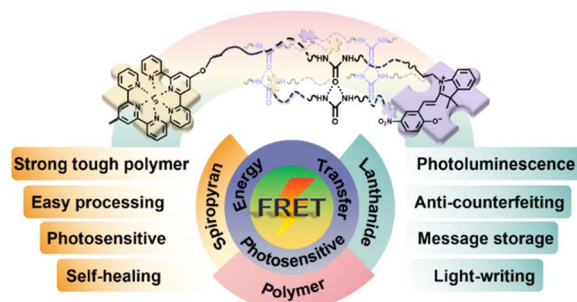
Zhenwei Wu, Xi Yang, Fangqing Zhang, Yangbin Liu* and Xiaoming Feng*



13306

Self-healing photoluminescent polymers with photosensitive behavior for information storage and multiple-level dynamic encryption

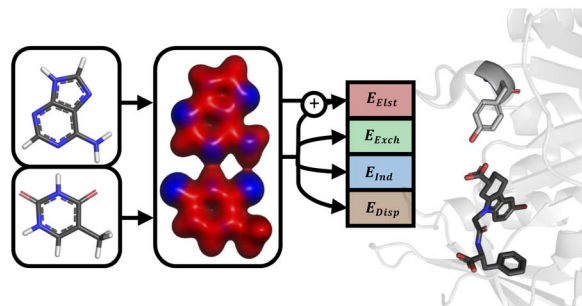
Di Zhao, Xianglong Li, Qianrui Li, Chunmei Yue, Yige Wang* and Huanrong Li*



13313

A physics-aware neural network for protein–ligand interactions with quantum chemical accuracy

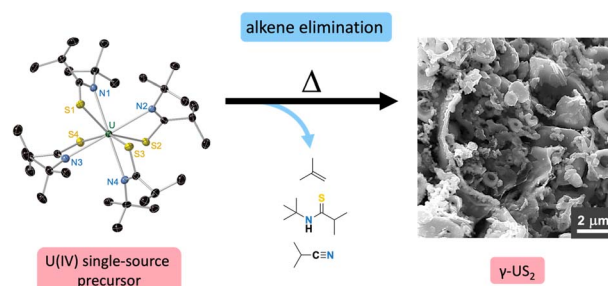
Zachary L. Glick, Derek P. Metcalf, Caroline S. Glick, Steven A. Spronk, Alexios Koutsoukas, Daniel L. Cheney and C. David Sherrill*



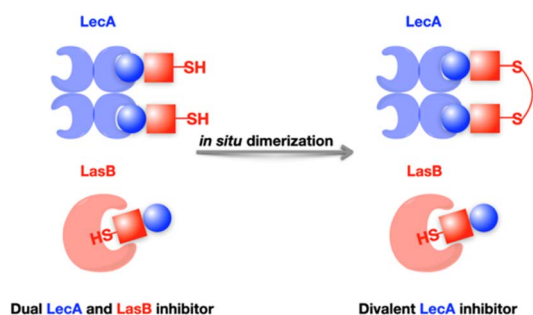
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Formation of uranium disulfide from a uranium thioamidate single-source precursor

Sheridon N. Kelly, Dominic R. Russo, Erik T. Ouellette, Debashree Roy, Andrew J. Swift, Michael A. Boreen, Patrick W. Smith, Liane M. Moreau,* John Arnold* and Stefan G. Minasian*



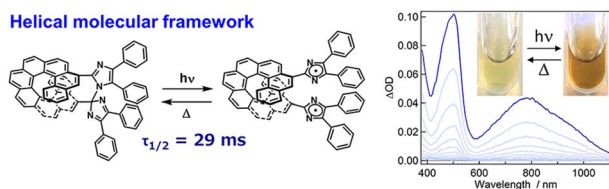
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Dual inhibitors of *Pseudomonas aeruginosa* virulence factors LecA and LasB

Olga Metelkina, Jelena Konstantinović, Andreas Klein, Roya Shafiei, Mario Fares, Alaa Alhayek, Samir Yahiaoui, Walid A. M. Elgaher, Jörg Haupenthal, Alexander Titz* and Anna K. H. Hirsch*

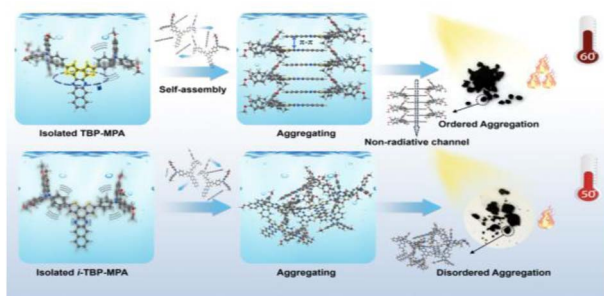
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Fast photochromism of helicene-bridged imidazole dimers

Katsuya Mutoh and Jiro Abe*

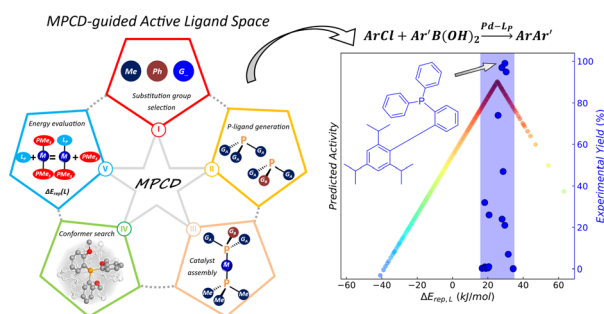
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Isomer engineering for deep understanding of aggregation-induced photothermal enhancement in conjugated systems

Peiyang Gu,* Tengfei He,* Zuoyu Wang, Shifan Wang, Liming Dong, Hanning Yao, Tao Jia,* Guankui Long, Guangfeng Liu and Hua Sun*

13359



Data-driven discovery of active phosphine ligand space for cross-coupling reactions

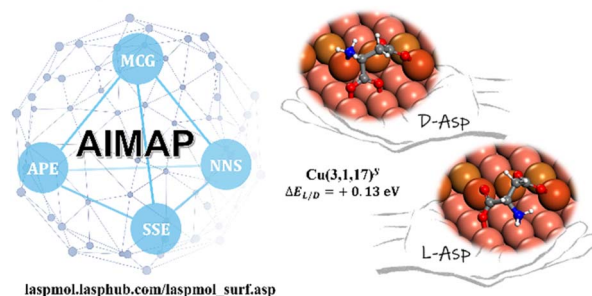
Sicong Ma,* Yanwei Cao, Yun-Fei Shi, Cheng Shang, Lin He* and Zhi-Pan Liu*



13369

Artificial intelligence driven molecule adsorption prediction (AIMAP) applied to chirality recognition of amino acid adsorption on metals

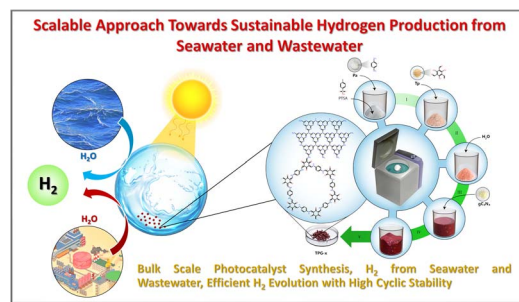
Zi-Xing Guo, Guo-Liang Song* and Zhi-Pan Liu*



13381

A scalable approach using a gC_3N_4 -covalent organic framework hybrid catalyst towards sustainable hydrogen production from seawater and wastewater

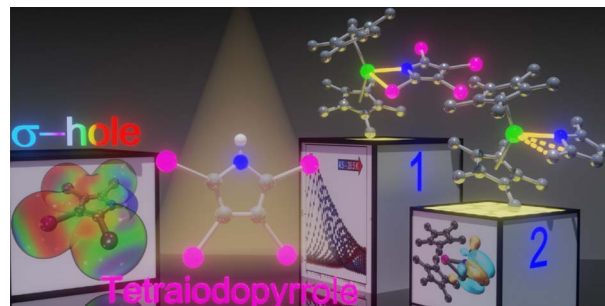
Kiran Asokan, T. M. Bhagyasree, George Devasia, Sailaja Krishnamurthy, Sabah Solim, Lina Rueda, Dhabia M. Al-Mohannadi, Mohammed Al-Hashimi, Konstantinos Kakosimos and Sukumaran Santhosh Babu*



13389

Construction of intermolecular σ -hole interactions in rare earth metallocene complexes using a 2,3,4,5-tetraiodopyrrolyl anion

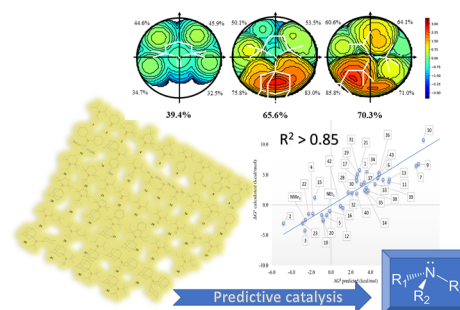
Francis Delano, IV, Florian Benner, Seoyun Jang, Samuel M. Greer and Selvan Demir*



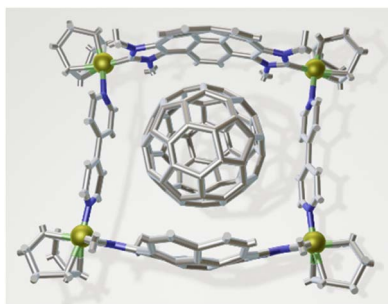
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Tuning the steric hindrance of alkylamines: a predictive model of steric editing of planar amines

Michele Tomasini, Maria Voccia, Lucia Caporaso, Michal Szostak* and Albert Poater*



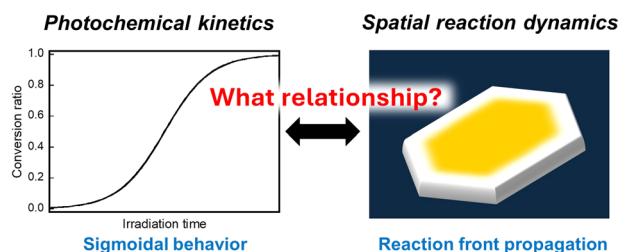
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A corannulene-based metallobox for the encapsulation of fullerenes

Susana Ibáñez,* Carmen Mejuto, Katherin Cerón, Pablo J. Sanz Miguel and Eduardo Peris*

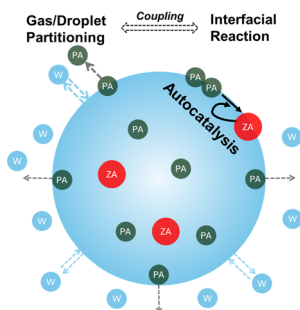
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Relationship between spatially heterogeneous reaction dynamics and photochemical kinetics in single crystals of anthracene derivatives

Sogo Kataoka, Daichi Kitagawa,* Hikaru Sotome, Syoji Ito, Hiroshi Miyasaka, Christopher J. Bardeen* and Seiya Kobatake*

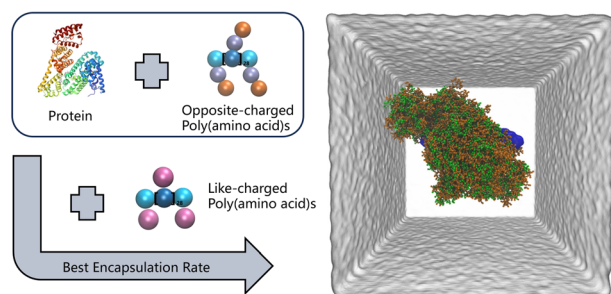
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Enhanced condensation kinetics in aqueous microdroplets driven by coupled surface reactions and gas-phase partitioning

Meng Li, Shu Yang, Meenal Rathi, Satish Kumar, Cari S. Dutcher* and Vicki H. Grassian*

13442



Unraveling mechanisms of protein encapsulation and release in coacervates via molecular dynamics and machine learning

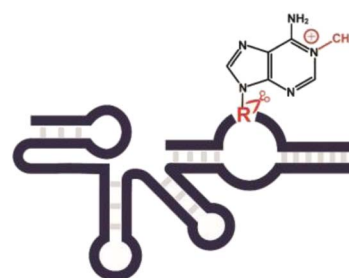
Yiwei Wang, Rongrong Zou, Ye qiang Zhou, Yi Zheng, Chuan Peng, Yang Liu,* Hong Tan, Qiang Fu and Mingming Ding*



13452

In vitro selection of *N*¹-methyladenosine-sensitive RNA-cleaving deoxyribozymes with 10⁵-fold selectivity over unmethylated RNA

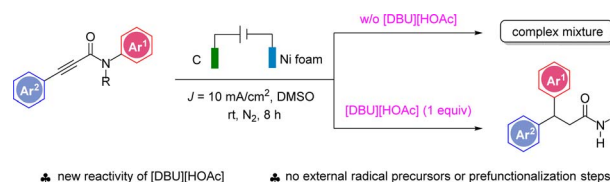
Jiarong Shi, Qiang Zhang, Yunping Wu, Yangyang Chang and Meng Liu*

m¹A-sensitive DNAzyme

13459

The merger of electro-reduction and hydrogen bonding activation for a radical Smiles rearrangement

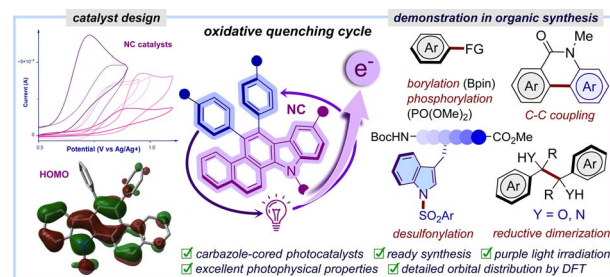
Liyuan Lan, Kun Xu* and Chengchu Zeng



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A toolbox approach to revealing a series of naphthocarbazoles to showcase photocatalytic reductive syntheses

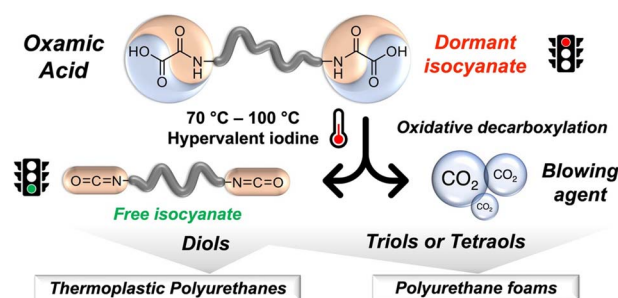
Sharmila Das, Samrat Kundu, Abhisek Metya and Modhu Sudan Maji*



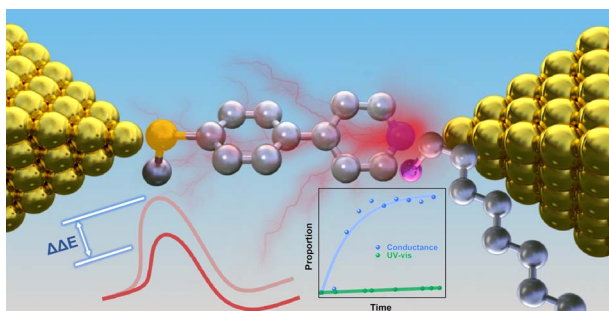
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Synthesis of polyurethanes through the oxidative decarboxylation of oxamic acids: a new gateway toward self-blown foams

Quentin Jaussaud, Ikechukwu Martin Ogbu, Govind Goroba Pawar, Etienne Grau, Frédéric Robert, Thomas Vidil, Yannick Landais* and Henri Cramail*



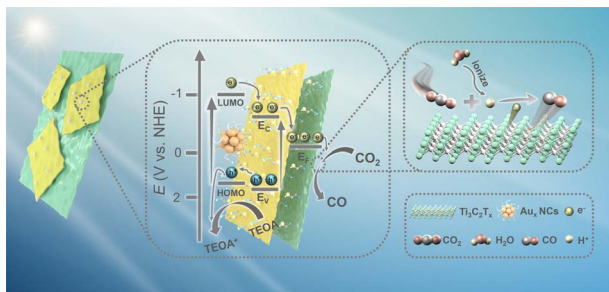
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Massive acceleration of S_N2 reaction using the oriented external electric field

Chun Tang, Meiling Su, Taige Lu, Jueting Zheng, Juejun Wang, Yu Zhou, Yu-Ling Zou, Wenqing Liu, Ruiyun Huang, Wei Xu, Lijue Chen, Yanxi Zhang, Jie Bai, Yang Yang, Jia Shi, Junyang Liu* and Wenjing Hong

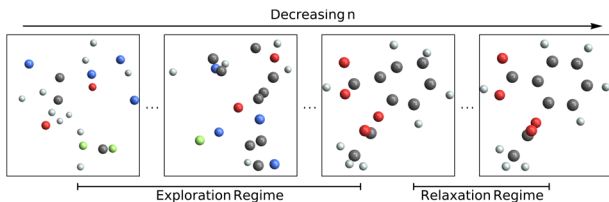
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Atomically precise metal nanoclusters combine with MXene towards solar CO_2 conversion

Yu-Shan Cai, Jia-Qi Chen, Peng Su, Xian Yan, Qing Chen, Yue Wu and Fang-Xing Xiao*

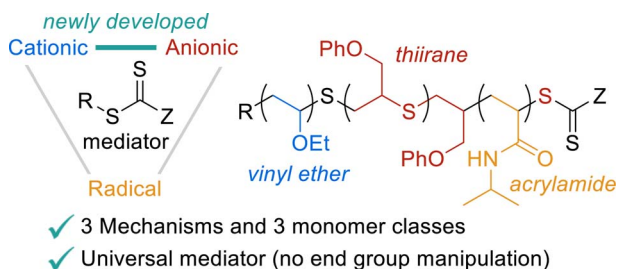
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Investigating the behavior of diffusion models for accelerating electronic structure calculations

Daniel Rothchild,* Andrew S. Rosen, Eric Taw, Connie Robinson, Joseph E. Gonzalez and Aditi S. Krishnapriyan*

13523



Combining photocontrolled-cationic and anionic-group-transfer polymerizations using a universal mediator: enabling access to two- and three-mechanism block copolymers

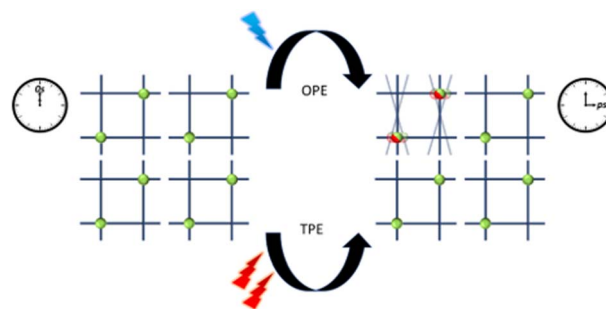
Brandon M. Hosford, William Ramos and Jessica R. Lamb*



13531

Out-of-equilibrium dynamics of a grid-like Fe(II) spin crossover dimer triggered by a two-photon excitation

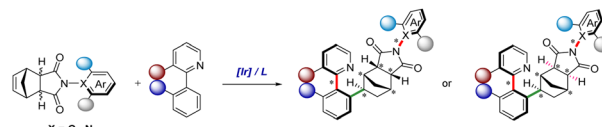
Jose de Jesus Velazquez-Garcia,* Krishnayan Basuroy, Joanne Wong, Serhiy Demeshko, Franc Meyer, Insik Kim, Robert Henning, Yannic U. Staechelin, Holger Lange and Simone Techert*



13541

Access to distal biaxial atropisomers by iridium catalyzed asymmetric C–H alkylation

Xueqing Hu, Yunxu Zhao, Tong He, Caoyue Niu, Feipeng Liu, Wei Jia, Yi Mu, Xingwei Li* and Zi-Qiang Rong*



- 100% atom economy
- up to 99% ee, >20:1 dr

- 59 examples, CPL-activity
- Distal diaxes (C–C and C–N/N–N)

1 synthetic step = 1 bond + 2 distal chiral axes + 5 chiral carbon centers

13550

A versatile fluorinated azamacrocyclic chelator enabling ¹⁸F PET or ¹⁹F MRI: a first step towards new multimodal and smart contrast agents

Charline Sire, Vincent Meneyrol, Nathalie Saffon-Merceron, Enzo Terreno, Francesca Garello, Lorenzo Tei, Emmanuelle Jestin, Raphaël Tripier and Thibault Troadec*

