

# Chemical Science

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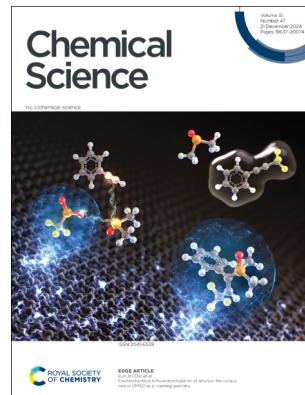
## IN THIS ISSUE

ISSN 2041-6539 CODEN CSHCBM 15(47) 19637–20074 (2024)



### Cover

See Sung Ho Jung, Jong Hwa Jung et al., pp. 19729–19738.  
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### Inside cover

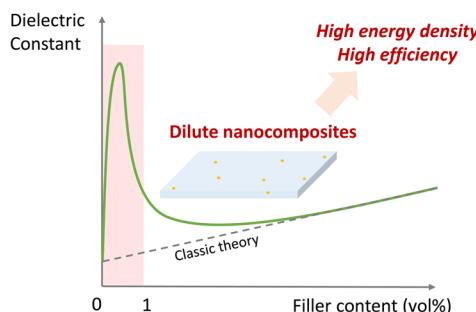
See Eun Jin Cho et al., pp. 19739–19744. Image reproduced by permission of Eun Jin Cho and Jihoon Jang from *Chem. Sci.*, 2024, 15, 19739.

## PERSPECTIVE

19651

### Dilute nanocomposites for capacitive energy storage: progress, challenges and prospects

Li Li, Wenhan Xu, Guanchun Rui, Shixian Zhang, Q. M. Zhang and Qing Wang\*

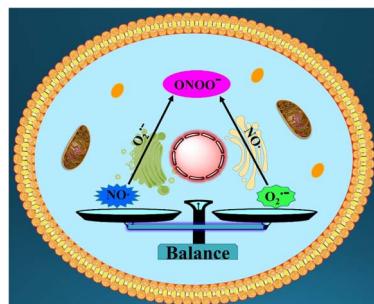


## REVIEWS

19669

### Recent progress in small-molecule fluorescent probes for the detection of superoxide anion, nitric oxide, and peroxy nitrite anion in biological systems

Yongqing Zhou, Xuan Kuang, Xiaofeng Yang, Juan Li, Xianzhe Wei, Won Jun Jang, Shan-Shan Zhang,\* Mei Yan\* and Juyoung Yoon\*



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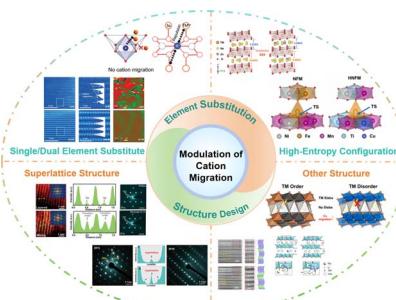
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## REVIEWS

19698

**Cation migration in layered oxide cathodes for sodium-ion batteries: fundamental failure mechanisms and practical modulation strategies**

Zhuang-Chun Jian, Jun-Xu Guo, Yi-Feng Liu, Yan-Fang Zhu,\* Jingqiang Wang\* and Yao Xiao\*

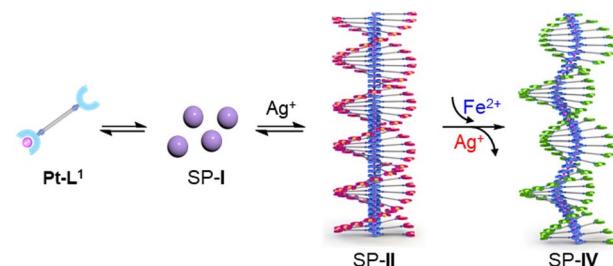


## EDGE ARTICLES

19729

**Pathway control in metallocsupramolecular polymerization of a monoalkynylplatinum(II) terpyridine complex through competitive complex formation**

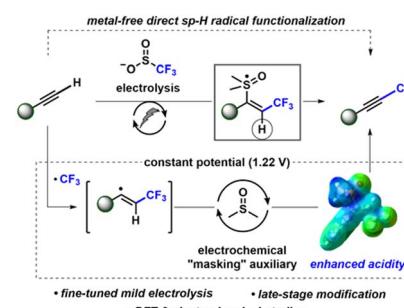
Minhye Kim, Heekyoung Choi, Minjoo Kim, Seonghan Kim, Seohyeon Yun, Eunji Lee, Jaeheung Cho, Sung Ho Jung\* and Jong Hwa Jung\*



19739

**Electrochemical trifluoromethylation of alkynes: the unique role of DMSO as a masking auxiliary**

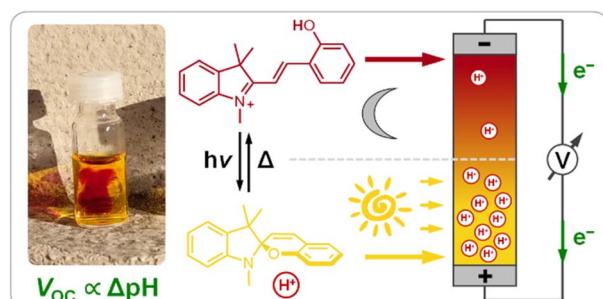
Jihoon Jang, Ho Seong Hwang, Haeryeong Jeong and Eun Jin Cho\*



19745

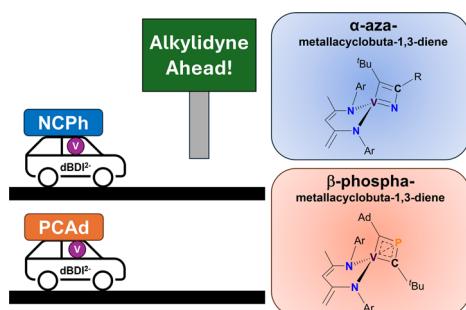
**Wiring proton gradients for energy conversion**

Xinchen Dai, Cesare Berton, Dong Jun Kim\* and Cristian Pezzato\*



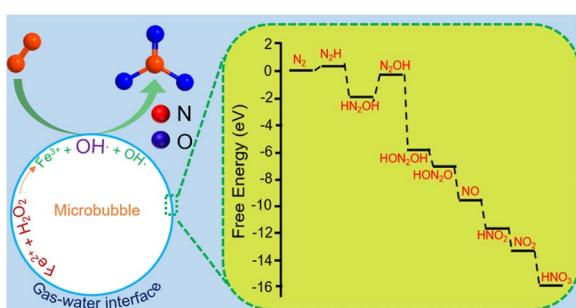
## EDGE ARTICLES

19752

**Pnictogen-based vanadacyclobutadiene complexes**

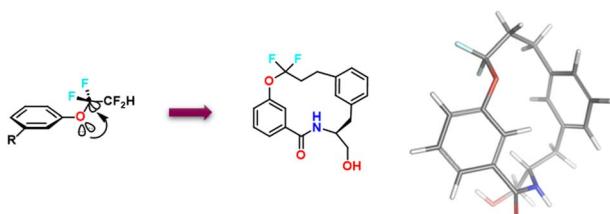
Mehrafshan G. Jafari, John B. Russell, Hwan Myung, Seongyeon Kwon, Patrick J. Carroll, Michael R. Gau, Mu-Hyun Baik\* and Daniel J. Mindiola\*

19764

**Understanding the formation of nitrate from nitrogen at the interface of gas–water microbubbles**

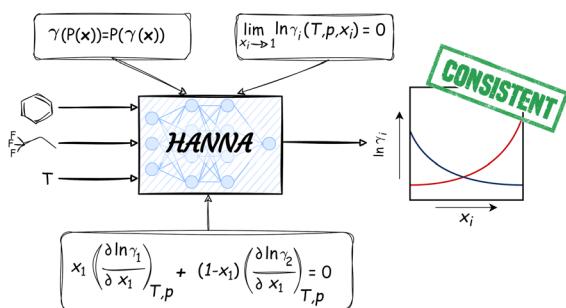
Sandeep Bose, Yu Xia\* and Richard N. Zare\*

19770

**The effect of gem-difluorination on the conformation and properties of a model macrocyclic system**

T. J. Cogswell,\* R. J. Lewis, C. Sköld, A. Nordqvist, M. Ahlqvist and L. Knerr\*

19777

**HANNA: hard-constraint neural network for consistent activity coefficient prediction**

Thomas Specht, Mayank Nagda, Sophie Fellenz, Stephan Mandt, Hans Hasse and Fabian Jirasek\*

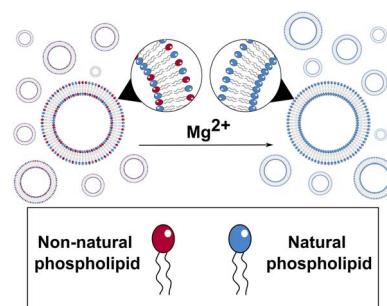


## EDGE ARTICLES

19787

**Mg<sup>2+</sup>-driven selection of natural phosphatidic acids in primitive membranes**

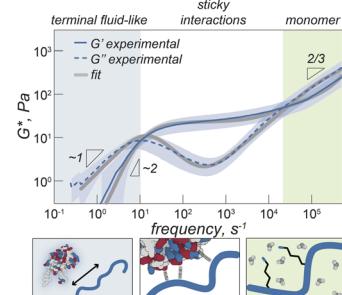
Krishnakavya Thaipurayil Madanan, Yuhan Li,  
Valeria J. Boide-Trujillo, David A. Russell  
and Claudia Bonfio\*



19795

**Viscoelasticity of globular protein-based biomolecular condensates**

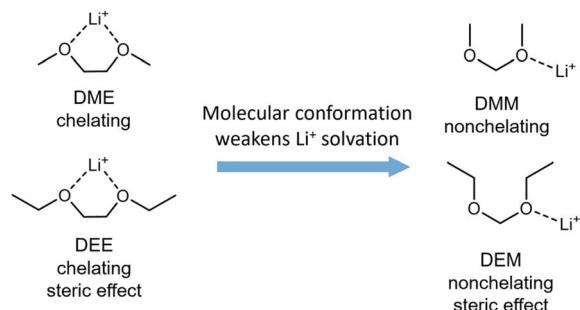
Rachel S. Fisher and Allie C. Obermeyer\*



19805

**Hyperconjugation-controlled molecular conformation weakens lithium-ion solvation and stabilizes lithium metal anodes**

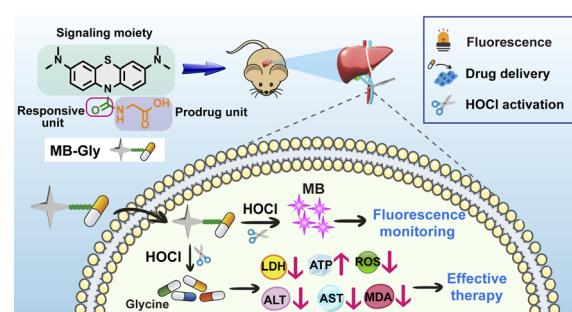
Yuelang Chen, Sheng-Lun Liao, Huaxin Gong,  
Zewen Zhang, Zhuojun Huang, Sang Cheol Kim,  
Elizabeth Zhang, Hao Lyu, Weilai Yu, Yangju Lin,  
Philaphon Sayavong, Yi Cui,\* Jian Qin\* and Zhenan Bao\*



19820

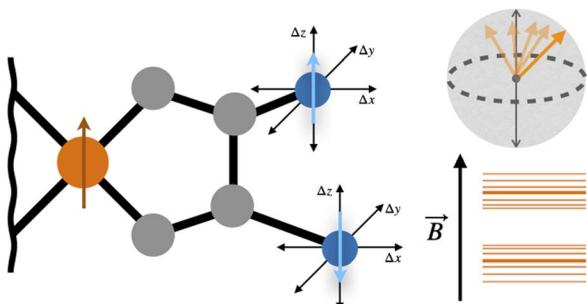
**A multifunctional “three-in-one” fluorescent theranostic system for hepatic ischemia–reperfusion injury**

Jihong Liu, Dongni Yin, Wen Zhang,\* Xin Wang,  
Tony D. James,\* Ping Li\* and Bo Tang\*



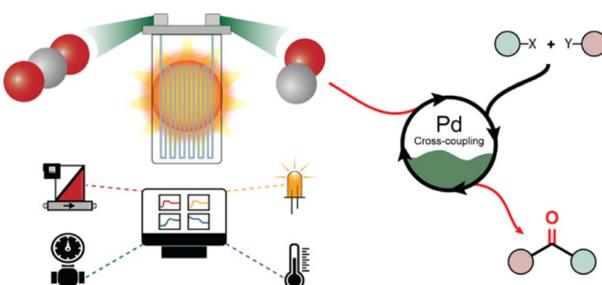
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19834


**Low temperature decoherence dynamics in molecular spin systems using the Lindblad master equation**

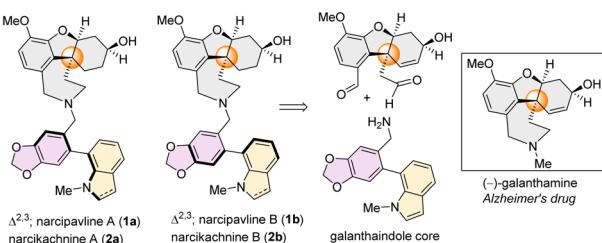
Timothy J. Krogmeier, Anthony W. Schlimgen and Kade Head-Marsden\*

19842


**Light-assisted carbon dioxide reduction in an automated photoreactor system coupled to carbonylation chemistry**

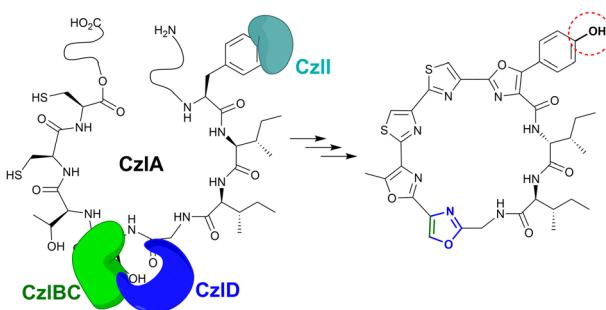
Jasper H. A. Schuurmans, Tom M. Masson, Stefan D. A. Zondag, Simone Pilon, Nicola Bragato, Miguel Claros, Tim den Hartog, Francesc Sastre, Jonathan van den Ham, Pascal Buskens, Giulia Fiorani and Timothy Noël\*

19851


**Total synthesis of atropodiastereomers of heterodimeric Amaryllidaceae alkaloids: narcipavline and narcikachnime**

Souvik Pal, Satyajit Majumder, Sovan Niyogi, Pranay Shyamal, Debabrata Mondal, Bishnu Das and Alakesh Bisai\*

19858


**Analysis of the cryptic biosynthetic gene cluster encoding the RiPP curacozole reveals a phenylalanine-specific peptide hydroxylase**

Samantha Hollands, Julia Tasch, David J. Simon, Dimah Wassouf, Isobel Barber, Arne Gessner, Andreas Bechthold and David L. Zechel\*

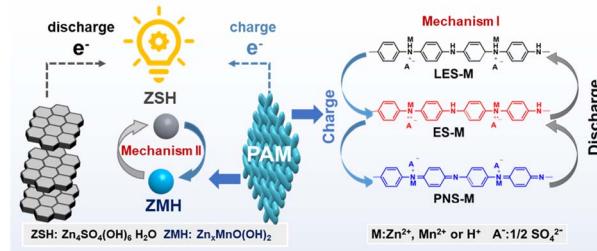


## EDGE ARTICLES

19870

**An interactive dual energy storage mechanism boosts high-performance aqueous zinc-ion batteries**

Shengen Gong, Meihua Zhu, Yan Zhou, Runan Li, Jianhua Zhang, Xiaoteng Jia,\* Danming Chao\* and Caiyun Wang\*



19886

**Organic dopant cyclization and significantly improved RTP properties**

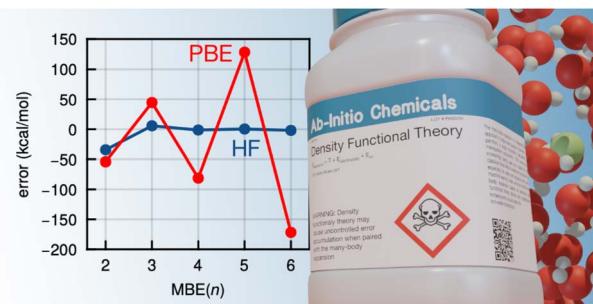
Shiguo Zhang, Guanyu Liu, Zhichao Mao, Shanfeng Xue, Qikun Sun\* and Wenjun Yang\*



19893

**Delocalization error poisons the density-functional many-body expansion**

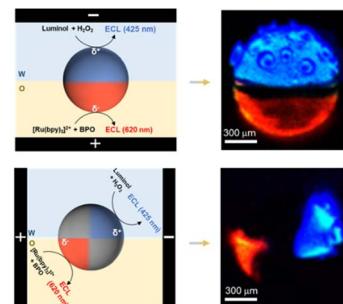
Dustin R. Broderick and John M. Herbert\*



19907

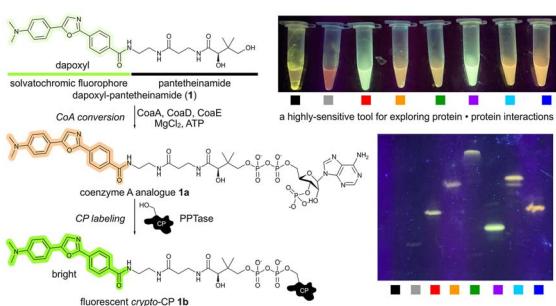
**Bipolar electrochemiluminescence at the water/organic interface**

Yuheng Fu, Bingbing Xie, Miaoxia Liu, Shaojuan Hou, Qunyan Zhu, Alexander Kuhn, Lin Zhang,\* Wensheng Yang\* and Neso Sojic\*

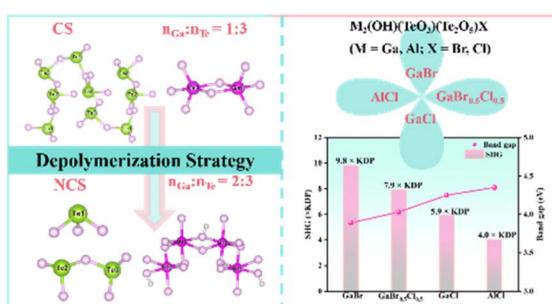


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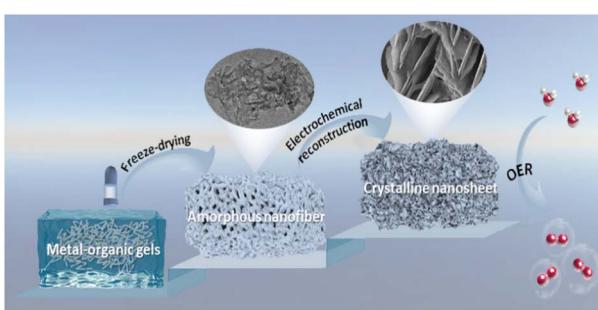
19913

**Differentiating carrier protein interactions in biosynthetic pathways using dapoxyl solvatochromism**Matthew G. Miyada, Yuran Choi, Kyle Rich,  
James J. La Clair and Michael D. Burkart\*

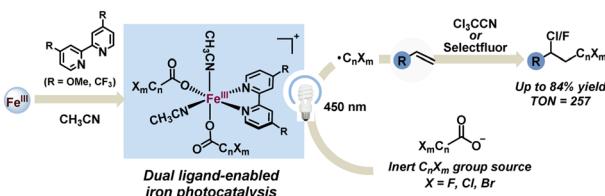
19920

**Noncentrosymmetric tellurite halides created by a depolymerization strategy: toward strong SHG intensity and wide bandgap**Dan-Dan Zhou, Chun-Li Hu, Xin-Wei Zhang,  
Jiang-Gao Mao and Fang Kong\*

19928

**Electrochemical reconstruction of metal-organic gels into crystalline oxy-hydroxide heterostructures for efficient oxygen evolution electrocatalysis**Kang Liu, Haikuo Lan, Yuting Chen, Weicheng Tang,  
Zhenyu Xiao, Yunmei Du, Jun Xing, Zexing Wu  
and Lei Wang\*

19936

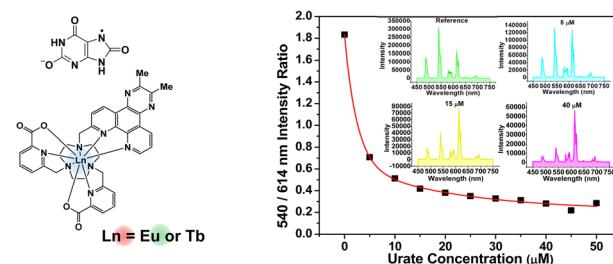
**Dual ligand-enabled iron and halogen-containing carboxylate-based photocatalysis for chloro/fluoro-polyhaloalkylation of alkenes**Wanru Han, Zhenyan Zhao, Kui Jiang, Yu Lan,\* Xuehan Yu,  
Xiaoyu Jiang, Wei Yang, Donghui Wei,\* Shi-Jun Li\*  
and Linbin Niu\*

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19944

**Mechanism of action and evaluation of ratiometric probes for uric acid using lanthanide complexes with tetraazatriphenylene sensitizers**

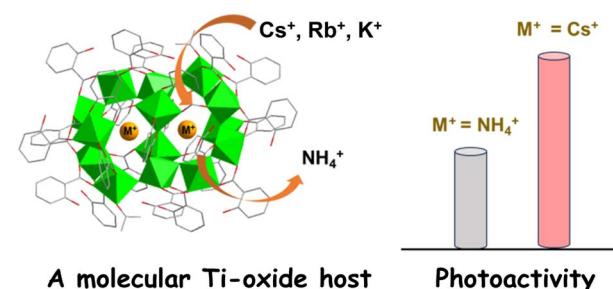
Xinyi Wen, Huishan Li, Zhijie Ju, Renren Deng and David Parker\*



19952

**Guest modulating the photoactivity of a titanium-oxide cage**

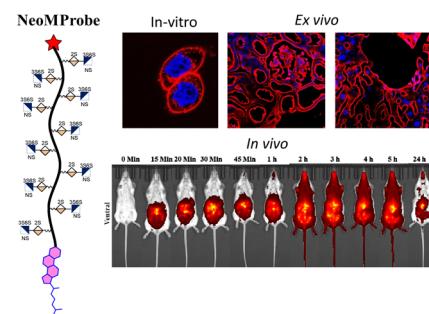
Dexin Wang, Yanshu Liu, Guanyun Zhang,\* Menghui Chu, Fangfang Gao, Guanjie Chen, Guo Wang, Chen-Ho Tung and Yifeng Wang\*



19962

**NeoMProbe: a new class of fluorescent cellular and tissue membrane probe**

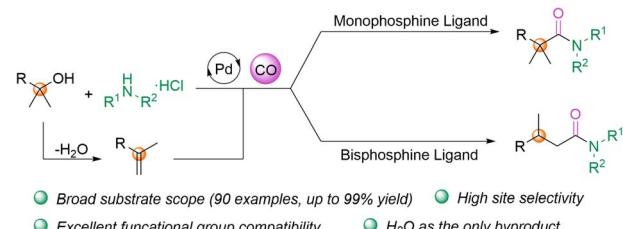
Saurabh Anand, Preeti Ravindra Bhoge, Rakesh Raigawali, Srinivas Vinod Saladi\* and Raghavendra Kikkeri\*



19970

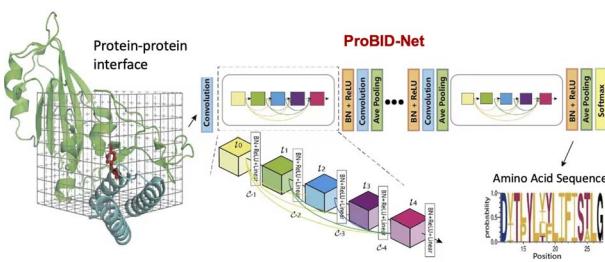
**Ligand-controlled palladium-catalyzed regiodivergent aminocarbonylation of tert-alcohols**

Xing-Wei Gu, Yan-Hua Zhao and Xiao-Feng Wu\*

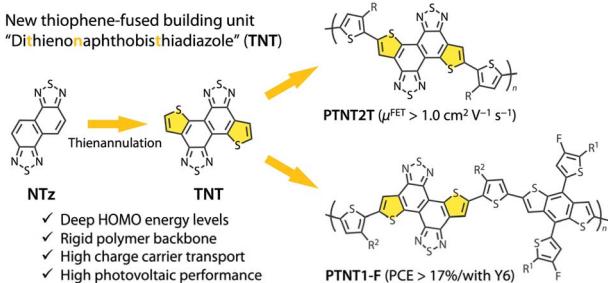


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19977

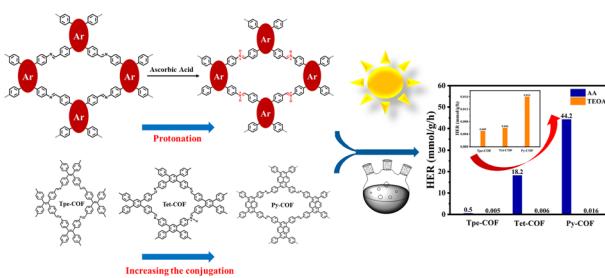


19991

**ProBiD-Net: a deep learning model for protein–protein binding interface design**

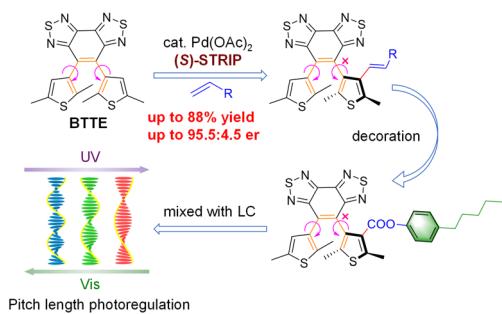
Zhihang Chen, Menglin Ji, Jie Qian, Zhe Zhang, Xiangying Zhang, Haotian Gao, Haojie Wang, Renxiao Wang\* and Yifei Qi\*

20002

**Double enhancement of protonation and conjugation in donor-imine-donor covalent organic frameworks for photocatalytic hydrogen evolution**

Huan He, Rongchen Shen, Yuhao Yan, Dejun Chen, Zhixiong Liu, Lei Hao, Xin Zhang\*, Peng Zhang\* and Xin Li\*

20013

**Pd(II)-catalyzed enantioselective C–H olefination and photoregulation of sterically hindered diarylethenes**

Guanlun Zhang, Xu Wu, Shiyu Mao, Mengqi Li\*, Honglong Hu, Bing-Feng Shi\* and Wei-Hong Zhu\*

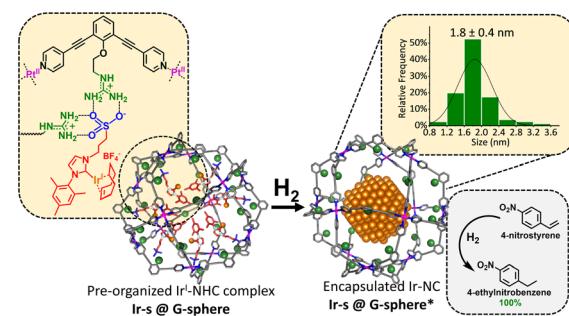


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20022

**M<sub>12</sub>L<sub>24</sub> nanospheres as supramolecular templates for the controlled synthesis of Ir-nanoclusters and their use in the chemo-selective hydrogenation of nitro styrene**

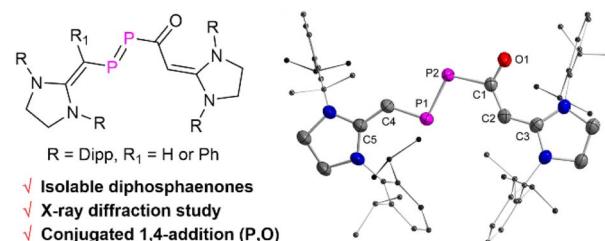
Lotte L. Metz, Rens Ham, Eduard O. Bobylev, Kelly J. H. Brouwer, Alfons van Blaaderen, Rim C. J. van de Poll, Victor R. Drozhzhin, Emiel J. M. Hensen and Joost N. H. Reek\*



20030

**Diphosphphaenones: beyond the phosphorus analogue of enones**

Jieli Lin, Shihua Liu, Shunlin Zheng, Hansjörg Grützmacher, Cheng-Yong Su and Zhongshu Li\*



20039

**Deep learning enabled ultra-high quality NMR chemical shift resolved spectra**

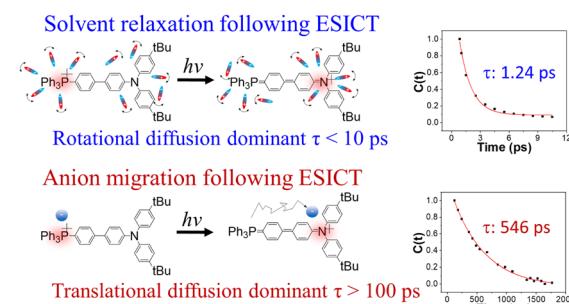
Zhengxian Yang, Weigang Cai, Wen Zhu, Xiaoxu Zheng, Xiaoqi Shi, Mengjie Qiu, Zhong Chen, Maili Liu and Yanqin Lin\*



20045

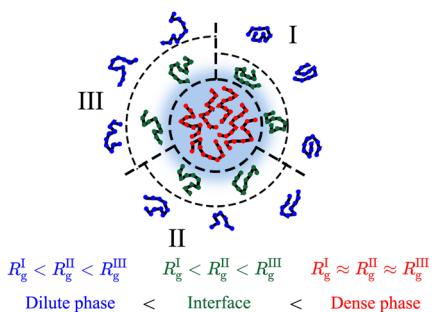
**Insights into the photoinduced anion translocation of donor-π-acceptor<sup>+</sup>(ion)<sup>-</sup> molecules**

Hao-Ting Qu, Iida Partanen, Kai-Hsin Chang, Yan-Ding Lin, Igor O. Koshevoy,\* Andrey Belyaev\* and Pi-Tai Chou\*



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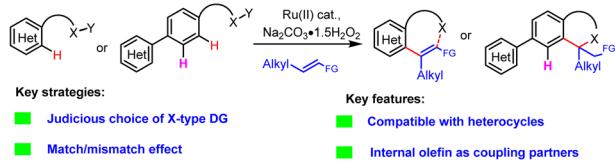
20056

**Sequence-dependent conformational transitions of disordered proteins during condensation**

Jiahui Wang, Dinesh Sundaravadivelu Devarajan, Keerthivasan Muthukumar, Young C. Kim,\* Arash Nikoubashman\* and Jeetain Mittal\*

20064

Regioselective oxidative Heck reaction of heterocycles with internal olefins:

**Ru(II)-catalyzed regioselective oxidative Heck reaction with internal olefins that tolerated strongly coordinating heterocycles**

Ci Chen, Qiaoya Zhang, Zhiwei Huang, Wensen Ouyang, Yang Gao, Jiye Luo, Yuan Liu, Yanping Huo, Qian Chen and Xianwei Li\*

