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## IN THIS ISSUE

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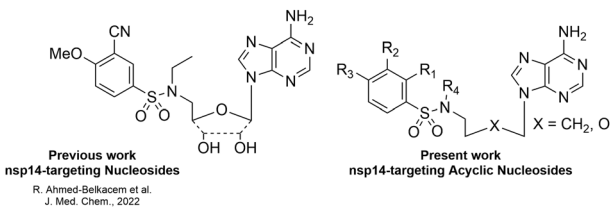
**Cover**
See Cedric Mongin, Stephane Aloise *et al.*, pp. 17711–17721. Image reproduced by permission of Stéphane Aloïse from *New J. Chem.*, 2024, **48**, 17711. Background image obtained *via* Pixabay.

## COMMUNICATIONS

17692

**Synthesis of acyclic analogues of adenosine sulfonamides and their activity against RNA cap guanine *N*7-methyltransferase of SARS-CoV-2**

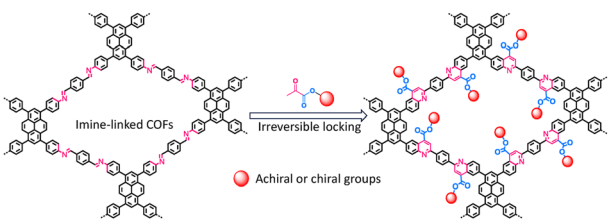
Rostom Ahmed-Belkacem, Adrien Delpal, Bruno Canard, Jean-Jacques Vasseur, Etienne Decroly* and Françoise Debart*




17696

**Construction of a quinoline-4-carboxylic ester linked covalent organic framework *via* Doebner–von Miller reaction**

Yuxing Tong, Ziwei Wang, Ben Liu, Chao Wan, Cheng Xu, Huaji Pang, Dekang Huang, Wenlong Zheng* and Yonggang Xiang*



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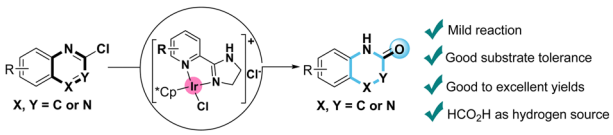
## COMMUNICATIONS

17700

**Successive hydrolysis and transfer hydrogenation of 2-chloroquinolines to 3,4-dihydroquinolones**

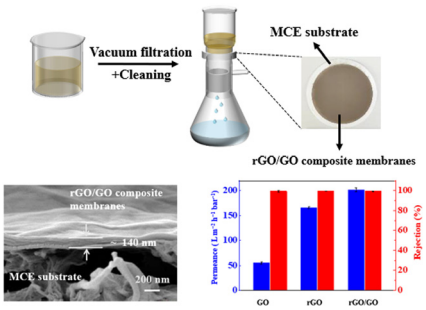
Renshi Luo, Sen Wang, Yuqiu Liang, Jianhua Liao and Lu Ouyang*




17706

**Ultrahigh water permeance of a composite reduced graphene oxide/graphene oxide membrane for efficient rejection of dyes**

Shanshan Liang,* Rujie Yang, Yingjie Di, Guangxiao Liu and Shujin Wu

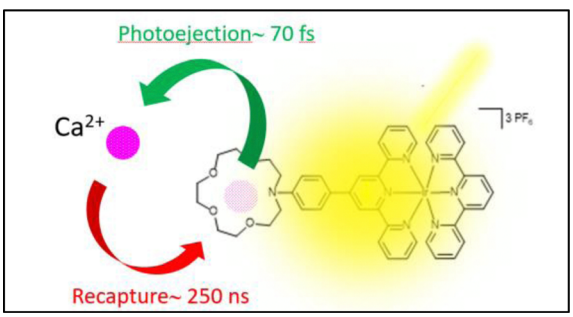



## PAPERS

17711

**Photoejection–recapture of the $Ca^{2+}$ cation studied by time resolved spectroscopy and TDDFT calculations: the case study of an azacrown–iridium(III) complex**

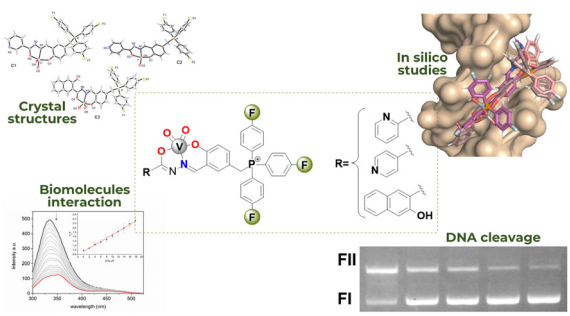
Clément Guerrin, Laure De Thieulloy, Julien Dubois, Clément Barois, Aurélie Perrier, Isabelle Leray, Cedric Mongin* and Stephane Aloise*




17722

**Zwitterionic dioxidovanadium(V) complexes containing fluorinated triphenylphosphonium ligands: structure and biomacromolecule studies**

Francisco Mainardi Martins, Daniele Cocco Durigon, Otávio Augusto Chaves, Rosely Aparecida Peralta, Davi Fernando Back* and Hernán Terenzi*



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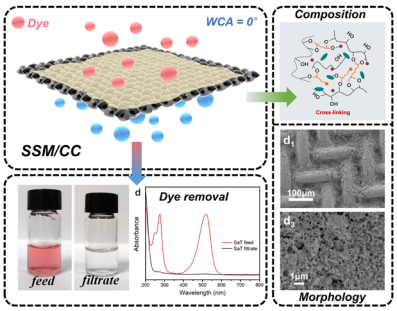
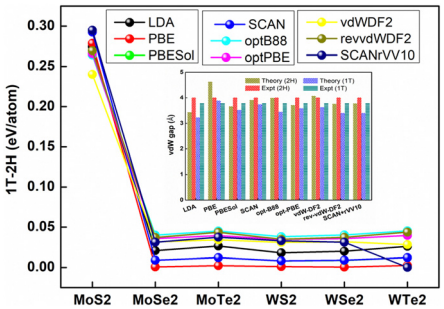
17734




**Brushing a superhydrophilic cross-linked coating on the metal mesh for dye separation**

Jun Zhang, Wei Li, Mingxiang Zheng, Jiawei Tan, Xinjuan Zeng,* Cailong Zhou,* Min Zhang and Lin Wang*

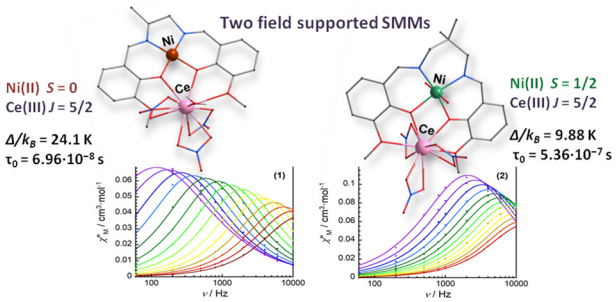
17742




**Structural characterization and functional assessment of exchange–correlation functionals in van der Waals TMDs $AB_2$ (A = Mo, W; B = S, Se, Te)**

Sushant Kumar Behera and Praveen C Ramamurthy*

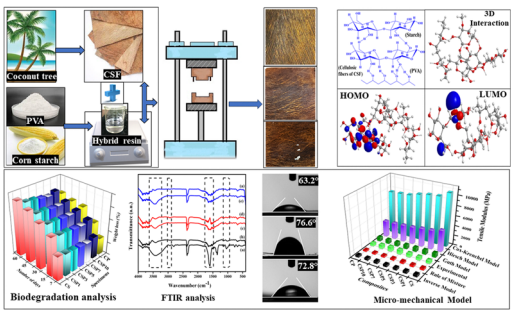
17750




**Two Ni/Ce complexes based on bicompartmental ligands with field supported slow magnetic relaxation**

Lenka Krešáková, Miroslava Litecká, Itziar Oyarzabal, Ján Titiš, Michaela Červeňáková, Elizabeth A. Hillard, Jerome Robert and Juraj Černák*

17761




**Fabrication and characterization of eco-friendly biocomposites from waste coconut spathe fabric for sustainable progress**

Diptiranjan Behera, Shruti S. Pattnaik, Sukanya Sanjibani, Ganesh C. Nayak, Nigamananda Das and Ajaya K. Behera*

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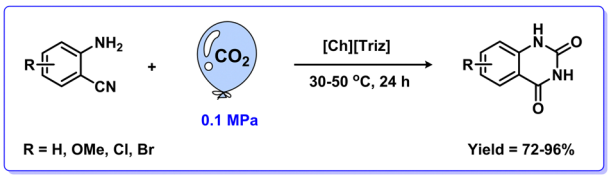
17773

**A bifunctional [Ch][Triz] ionic liquid catalyst for $CO_2$ transformation into quinazoline-2,4(1*H*,3*H*)-diones under mild conditions**

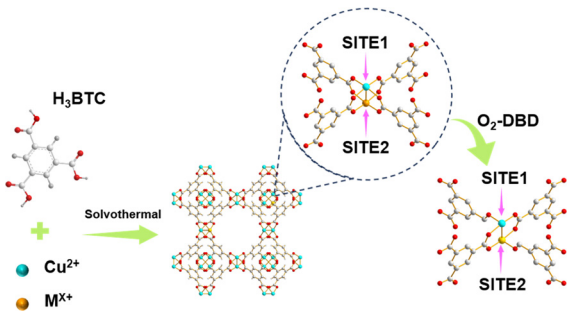
Xiang Gao,* Jiajia Zhao, Jiao Liu, Yuehua Deng, Ying Gao,* Fei Wang and Yanrui Li




17779

**Enhancement of electrocatalytic $CO_2$ performance by different components of Cu-based bimetallic MOFs**

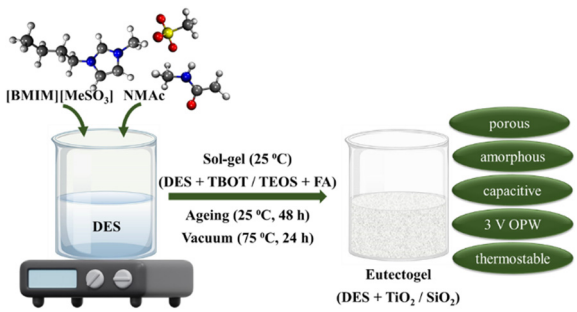
Jvwei Liu, Qiang Zhang,* Jianlin Wang, Conglin Chen, Shenjie Zhang, Fang Guo and Junqiang Xu




17787

**Novel eutectogels derived from an ionic-liquid-based deep eutectic solvent as electrolytes for supercapacitors: synthesis and characterization**

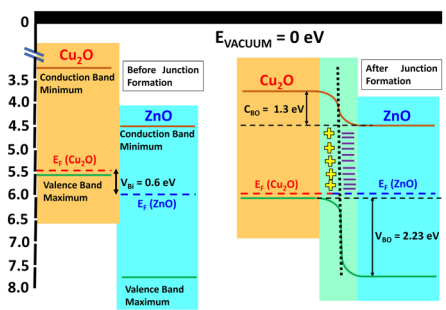
Arindam Dutta, Wade Millar, Debbie S. Silvester and Tamal Banerjee*




17802

**Photoelectrochemical performance of nanoscale $Cu_2O$ by integrating ZnO thin films mimicking a 3D–2D heterojunction: experiments & first-principles analysis**

Ajay, Chinmay Rakesh Shukla, Shubham Kumar, Pravin Popinand Ingole, Sameer Sapra and Sumant Upadhyay*



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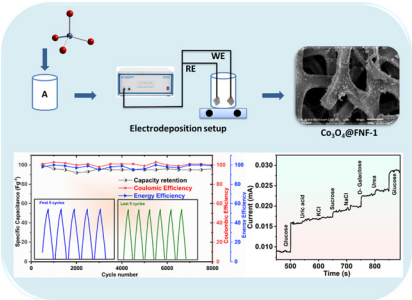
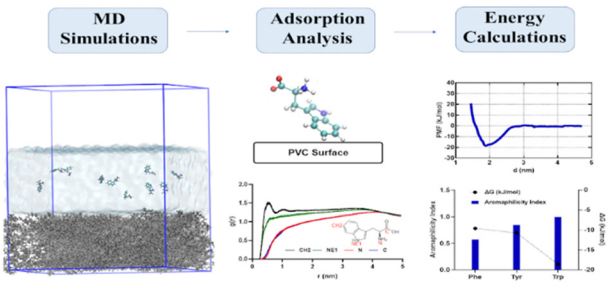
17812




**Facile growth of binder-free $Co_3O_4$@FNF electrode with superior electrochemical performance for energy storage and sensing applications**

Muhammad Owais Ameen, Ahtisham Abdul Wahid, Muhammad Usman,* Yasir A. Haleem,* Muhammad Asif Hussain, Kabeer Raza, Naseeb Ahmed, Abdul Ghafar Wattoo and Ishfaq Ahmad

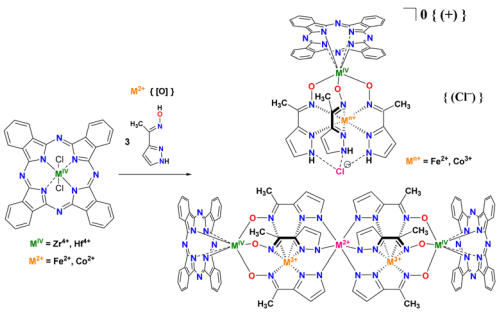
17822




**Deciphering amino acid adsorption on PVC surface: insights from molecular dynamics and PMF calculations**

Amr H. Saleh, Patrice Malfreyt and Mehdi Sahihi*

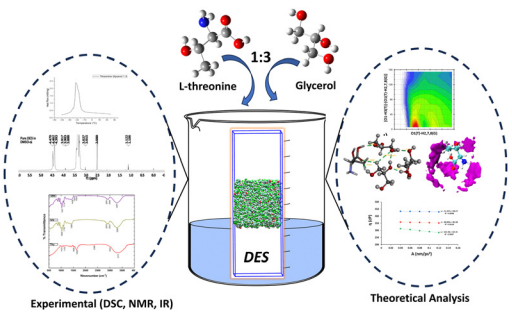
17831



**Synthesis, structure and spectroelectrochemistry of hybrid metal(IV)phthalocyaninato-capped 3d-metal pyrazoloximates as prospective precursors of stimuli-induced (responsive) single-molecule magnets, logic gates and qubits**

Svetlana A. Belova, Semyon V. Dudkin, Alexander S. Belov, Anastasia A. Danshina, Pavel V. Dorovatovskii, Yulia H. Budnikova, Vera V. Khrizanforova, Svetlana Yu. Bratskaya, Denis V. Balatskiy and Yan Z. Voloshin*

17849




**Physicochemical and structural investigation of L-threonine/glycerol-based deep eutectic solvents using experimental and molecular modelling approaches**

Md Jaish Uddin, Mahdi Ghasemi, Cladie B. White, Anusha Bhattarai, Hasina Akhter, Abdul Hannan, Carl Jacky Saint-Louis and Mohammad A. Halim*

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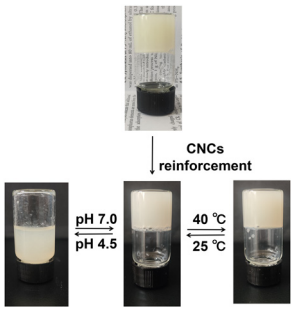
17865

**Cellulose nanocrystal-reinforced thermally responsive dynamic hydrogel**

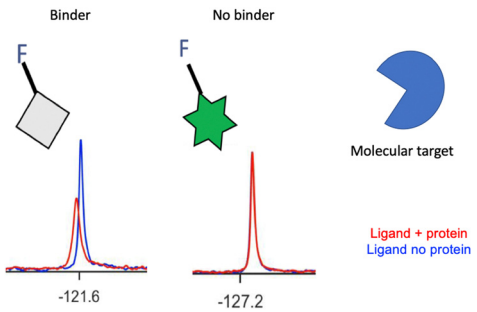
Long Yang,* Simei Zhang, Zemei Hu, Jing Li and Guangyin Xie




17872

**Synthesis of a thiophene-based fluorinated library applied to fragment-based drug discovery *via* $^{19}$F NMR with confirmed binding to mutant HRAS$^{G12V}$**

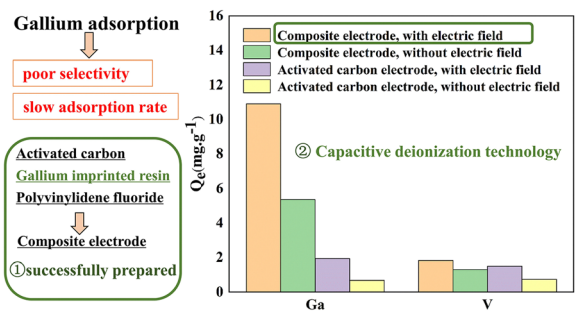
David Bendahan, Tanos C. C. Franca, Kathleen C. Amiens, Yann Ayotte, Pat Forgione and Steven R. LaPlante*




17878

**Preparation of a gallium-imprinted resin-capacitive deionization electrode and study of its gallium adsorption performance**

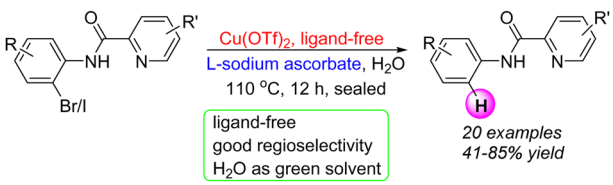
Song Wang, Guozhi Lv* and Tingan Zhang




17886

**L-Sodium ascorbate-promoted ligand-free Cu-catalyzed hydrodehalogenation of *o*-halopicolinanilides in water**

Yunhong Shen and Zewei Mao*



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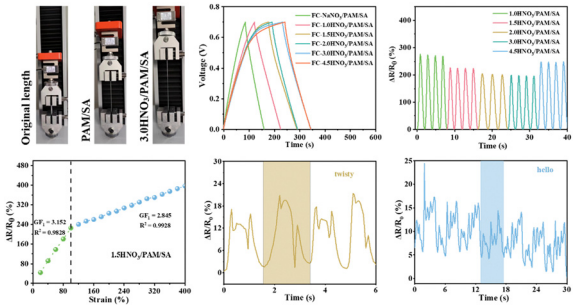
## PAPERS

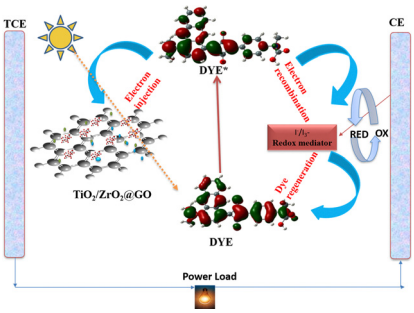
17891




### Stretchable and conductive polyacrylamide/sodium alginate dual-network hydrogels mediated by $HNO_3$ for flexible capacitors and wearable sensors

Xiang Liu, Weiyi Li, Ping Wang* and Zheng Xing

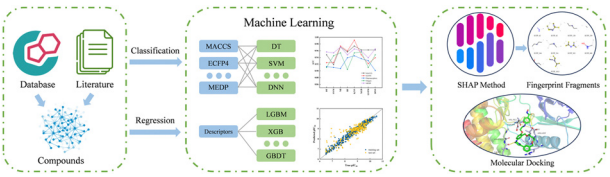
17900




### Unveiling the optoelectronic structure and photovoltaic potential of $ZrO_2$@GO through cosensitization with squaraine dye in DSSC: a computational study

Kaniz Fatima, Aaliya Qureashi, Irfan Nazir, Zia-ul-Haq, Firdous Ahmad Ganaie, Taniya Manzoor and Altaf Hussain Pandith*

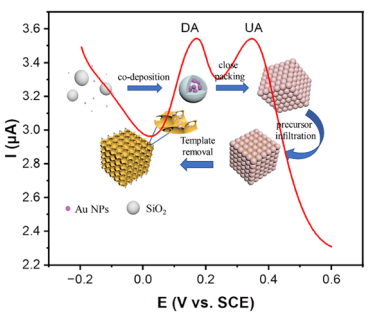
17915




### Investigation of dual JAK2 and HDAC6 inhibitors using machine learning methods

Yuquan Zhang and Yan Li*

17928




### Template-assisted synthesis of 3D ordered mesoporous graphitic carbon nitride decorated with gold nanoparticles for dopamine sensing

Yi Wang, Xiaoguang Sang, Jingce Bi, Hongjun Fu, Ningning Liu, Xia Zhang, Zhuopeng Wang and Yide Han*

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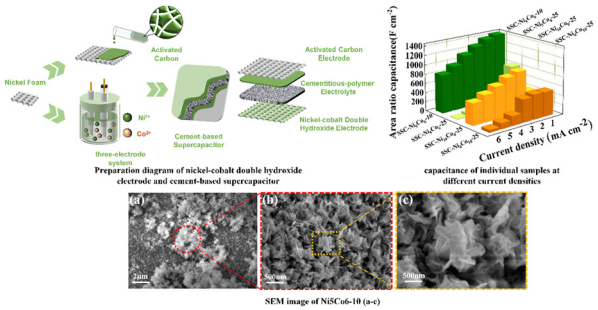
17935

**Improving the composite-structured supercapacitor assembled with Ni–Co-layered double hydroxide and polymer cement electrolyte through structural optimization**

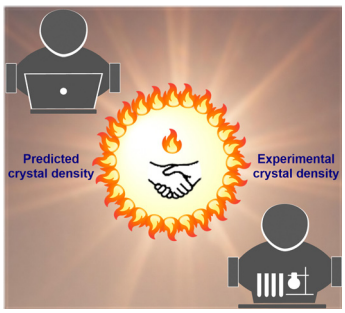
Lu Wang, Muyang Shi and Dong Zhang*




17947

**New approach for predicting crystal densities of energetic materials**

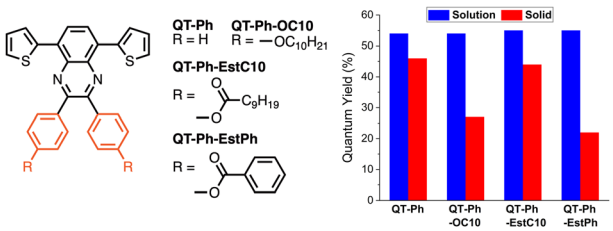
Sohan Lal, Haixiang Gao and Jean'ne M. Shreeve*




17953

**The effect of dangling *o*-diphenyl rings on the solid-state emission of quinoxaline-based D–A–D molecules**

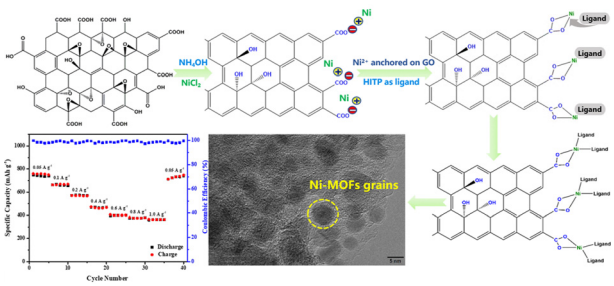
Marco S. Valverde Paredes and Dong-Chan Lee*




17961

**Excellent lithium storage performance of Ni-MOFs/GO composite as anode in lithium ion battery**

Weijie Zhu, Gaolei Wang, Shiqi Zhou, Yuxin Min, Chaofan Yang and Junjie Huang*



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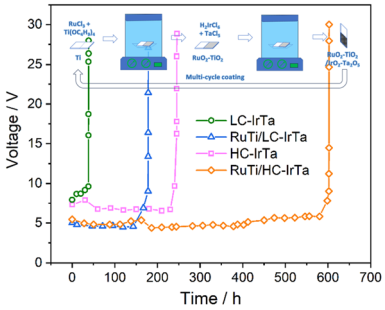
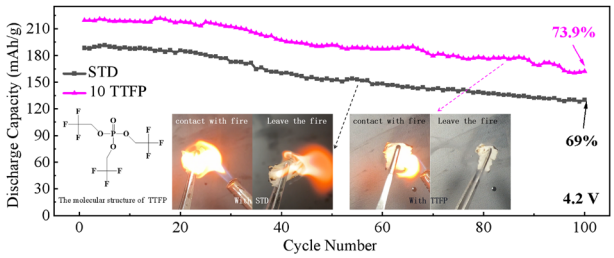
17969




## Improvement of chlorine evolution stability and activity of a $RuO_2$–$TiO_2$/$IrO_2$–$Ta_2O_5$ electrode with low iridium content through an alternate coating and thermal decomposition method

Lin Liu, Tianli Dong, Yuefei Xin, Zongxin Ye, Pengyi Zhao, Wenjing Gao, Huanhuan Tang, Ting Yin, Zhandong Ren* and Yuchan Zhu*

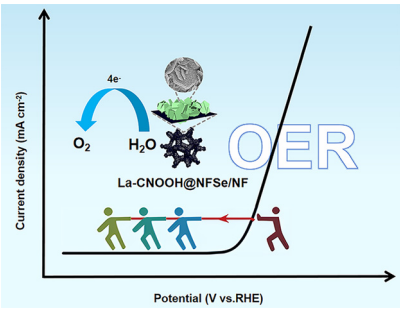
17978




## Tris(2,2,2-trifluoroethyl) phosphite (TTFP) as a flame-retardant co-solvent to improve the safety and electrochemical performances of lithium-ion batteries

Caixia Huang, Lucheng Li, Peng Yang and Jun Chen*

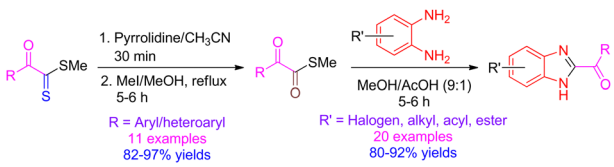
17990




## Regular pentagonal folded La doped CoNiOOH@FeSe@NiSe/NF nanosheet array for high efficiency alkaline electrocatalytic oxygen evolution reaction

Biaobiao Lu, Yaoxia Yang,* Yu Zhang, RuiRui Zhang, Fuxing Zhou, Qingtao Wang, Wei Zeng and Dongfei Sun

17998




## Cyclocondensation of *o*-phenylenediamines with α-ketothioesters: a novel approach for the synthesis of 2-acylbenzimidazoles

Kumar Kavya, Kanaka Vijayashankar Honnabandar, Bilagumba T. Sridhar, Toreshettahally R. Swaroop, Anantharaman Shivakumar and Kempegowda Mantelingu*

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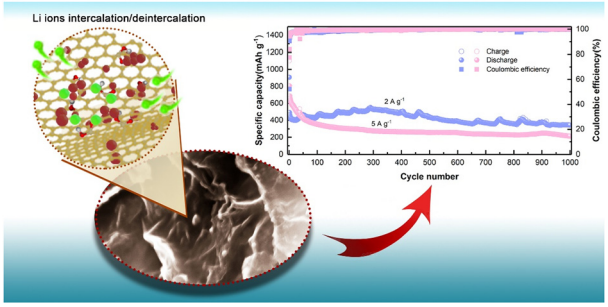
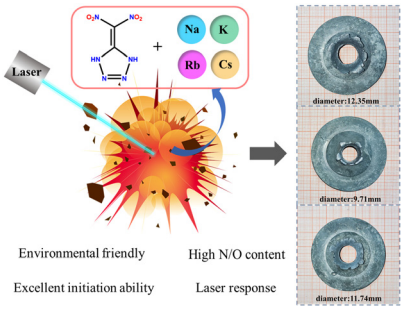
18004

**Self-assembly of a NiO@$NiFe_2O_4$/rGO architecture for stable and ultra-long-life lithium-ion storage**

Lihua Yao* and Linhua Yao




18014

**Dinitromethyltetrazole (DNMT)-based energetic coordination polymers (ECPs) as lead-free primary explosives and laser initiators**

Jinkun Guo, Shiliang Huang, Liyuan Wei, Qing Lang, Wenjia Hao, Yuangang Xu, Yu Liu* and Ming Lu*