# CrystEngComm

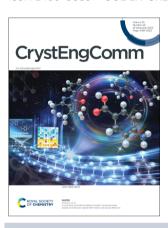
A journal at the forefront of the design and understanding of solid-state and crystalline materials

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# IN THIS ISSUE

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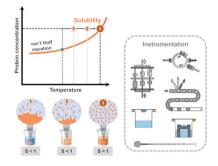
Cover See Zhong Li et al., pp. 6405-6415. Image reproduced by permission of Yanlei Kang from CrystEngComm, 2023, 25, 6405.

# **HIGHLIGHT**

## 6388

Advances in protein solubility and thermodynamics: quantification, instrumentation, and perspectives

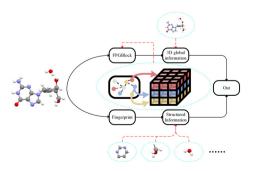
Joana Ferreira and Filipa Castro\*



# **PAPERS**

A cocrystal prediction method of graph neural networks based on molecular spatial information and global attention

Yanlei Kang, Jiahui Chen, Xiurong Hu, Yunliang Jiang and Zhong Li\*



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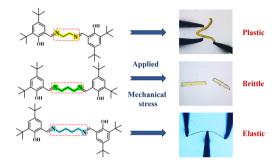
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# **PAPERS**

# 6416

# Linker size dependent mechanical properties of diimine based molecular crystals

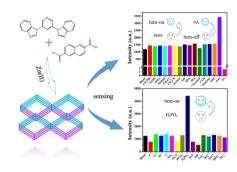
Deepak Manoharan, Shamim Ahmad, Srinu Tothadi, Franziska Emmerling, Biswajit Bhattacharya\* and Soumyajit Ghosh\*



# 6424

2D → 3D polycatenated Zn(II) metal-organic framework with good chemical stability as a fluorescent sensor toward salicylaldehyde, acetylacetone and H<sub>2</sub>PO<sub>4</sub>

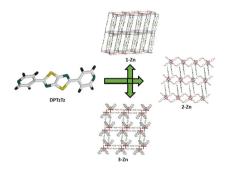
Ya-Ping Li,\* Jian-Hua Zhang, Xiao-Xia Zhang and Sui-Jun Liu\*



# 6434

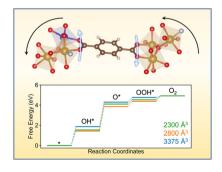
# The physical and electronic properties of Metal-**Organic Frameworks containing** dipyridylthiazolo[5,4-d]thiazole

Felix J. Rizzuto, Shyam C. Pal, Eleanor R. Kearns, Carol Hua, Marcello B. Solomon, Patrick W. Doheny, Thomas B. Faust, Cameron J. Kepert,\* Madhab C. Das\* and Deanna M. D'Alessandro\*



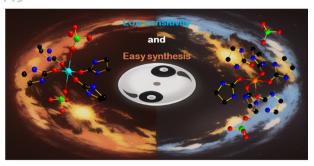
# Catalytic activities modulated by flexible bimetallic metal-organic frameworks

Xiang He\*



# **PAPERS**

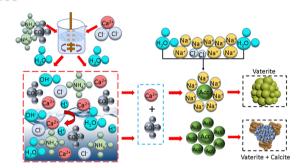
# 6449



# 2-Imidazolidone metal complexes: increased hydrogen bonds and fused ring ligand ratio to be insensitive

Baolong Kuang,\* Tingwei Wang,\* Chao Zhang, Han Zhang, Zujia Lu, Zhiming Xie, Meiqi Xu, Zhenxin Yi and Jianguo Zhang\*

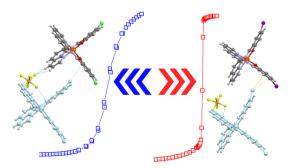
#### 6455



# Influence of Na<sup>+</sup> on vaterite formation, content and yield using steamed ammonia liquid waste as a calcium source

Xuewen Song,\* Xinrui Hua, Xiaomin Zhang,\* Yuxin Tuo, Yihan Su, Jianxiang Ma,\* Sicheng Mu, Tianxing Chen, Panyang He, Lianjing Ma and Cunjian Weng\*

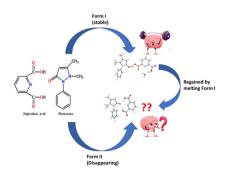
# 6472



# Structural features that modulate the sharpness of the spin crossover transition in [Fe<sup>III</sup>(5-X-qsal)<sub>2</sub>]<sup>+</sup> based salts

Bruno J. C. Vieira,\* Laura C. J. Pereira,\* Vasco da Gama and João C. Waerenborgh

# 6478



# In the pursuit of a 'disappearing' anhydrous phase of the antipyrine-dipicolinic acid (ANT-DPA) cocrystal: explained through relative stability and charge density analyses

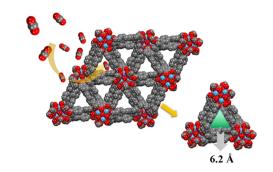
Sehrish Akram, Arshad Mehmood,\* Sajida Noureen and Magsood Ahmed\*

# **PAPERS**

#### 6489

A stable ultra-microporous hafnium-based metalorganic framework with high performance for CO<sub>2</sub> adsorption and separation

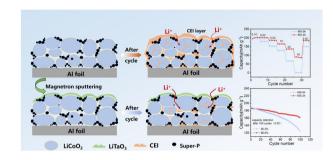
Yali Ma, Haitang Wang, Hailong Wang, Jiani Wang, Shuaiyu Jiang, Qiang Zheng, Songyan Jia, Xue Li\* and Tianyi Ma\*



# 6496

The improvement of the high voltage performance of LiCoO<sub>2</sub> by coating LiTaO<sub>3</sub> via magnetron sputtering

Chenhui Wang, Shaopeng Li, Weiyi Chen, Yining Zhao, Shu Xu, Hui Dou and Xiaogang Zhang\*



# 6503

Two isostructural complexes of Ni(II) and Zn(II) with violurate and pyridine: a detailed structural, theoretical, magnetic, and NMR investigation

Subhadip Roy, Susital Mal, Rupak Banik, Subrata Das,\* Ľubor Dlháň, Ján Titiš,\* Roman Boča, Alexander M. Kirillov,\* Alexander S. Novikov, Paul Hazendonk,\* Ray J. Butcher, Antonio Bauza and Antonio Frontera\*



Microwave-assisted hydrothermal solution process for accelerated formation of 3D hierarchical flowery anatase-TiO<sub>2</sub> microspheres with excellent photocatalytic activity

Praveen Kumar Lavudya, SuryaBindu Sesha Devarakonda, Harita Pant, Sarah Geo, Avijit Tudu, Vadali Venkata Satya Siva Srikanth and Rajanikanth Ammanabrolu\*

