

# MSDE

## Molecular Systems Design & Engineering rsc.li/molecular-engineering

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### IN THIS ISSUE

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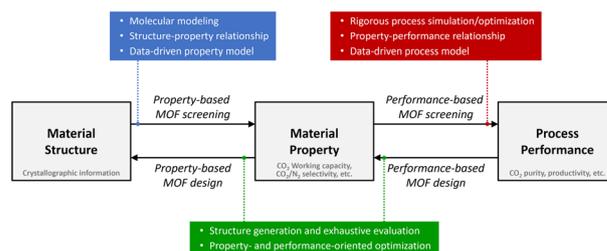
**Cover**  
See Takahiro Ichikawa et al.,  
pp. 1024–1027.  
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Syst. Des. Eng.*, 2025, 10, 1024.

### REVIEW

1005

#### Computer-aided metal–organic framework screening and design approaches toward efficient carbon capture processes

Zihao Wang and Teng Zhou\*

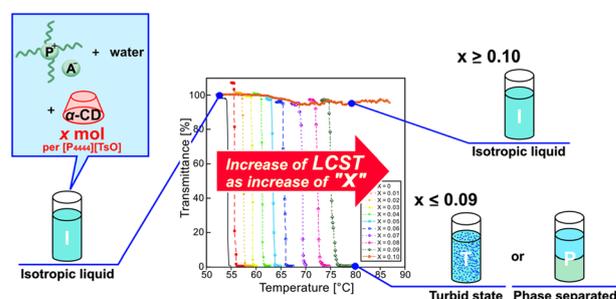


### COMMUNICATIONS

1024

#### Control of LCST phase transition behaviour of phosphonium-based ionic liquids in water using supramolecular host-guest chemistry

Saori Yamaguchi, Hiroyuki Ohno, Nobuhumi Nakamura and Takahiro Ichikawa\*





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1028

## Serinol as a tunable and sustainable framework for high capacity, low viscosity, water-lean CO<sub>2</sub> capture and switchable solvents

Jun Wang, Alain Tundidor Camba, Ifeanyi Samuel Ibeto, Zahra Sekhavat Pour, Joseph T. Danner, Steven T. Weinman, C. Heath Turner and Jason E. Bara\*

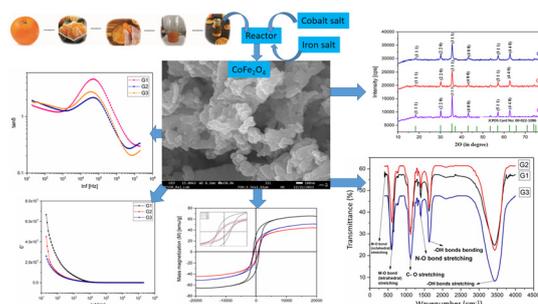


PAPERS

1034

## Green synthesis of nano cobalt ferrite for the enhancement of structural, morphological, magnetic, electrical, and optical properties

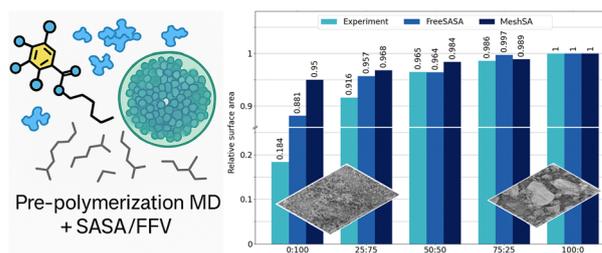
Afia Yasmin, Bristy Biswas, Md. Lutfor Rahman, Juliya Khanam, Rabeya jahan Rakhi, Dipa Islam, Md. Sahadat Hossain, Nahid Sharmin, Israt Jahan Lithi and Md. Farid Ahmed\*



1051

## Designing porous molecularly imprinted polymers via simulation of pre-polymerisation mixtures: a case study with trinitrotoluene

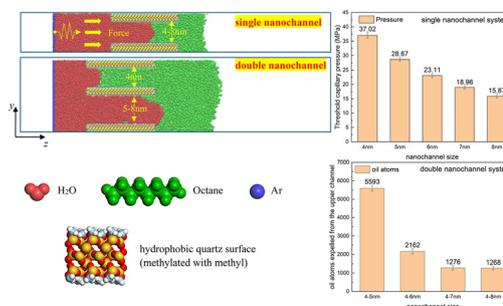
Jasmine C. Lightfoot, William Battell, Bernardo Castro-Dominguez and Carmelo Herdes\*



1060

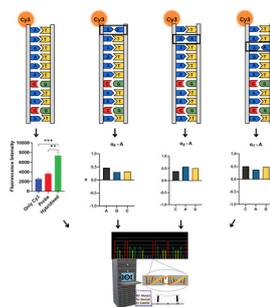
## Molecular dynamics simulation of oil–water flow behavior in single and double nanochannels

Chengen Zhao, Yuqi Liu, Zihao Guo, Weiming Wang, Youguo Yan and Lixia Zhou\*



## PAPERS

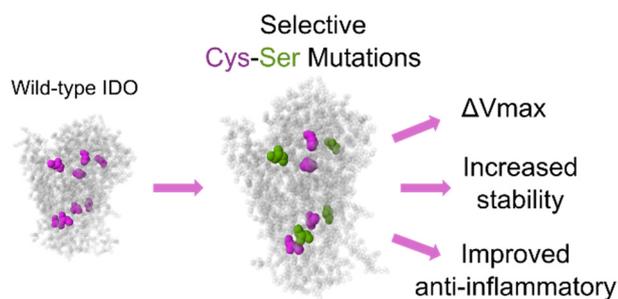
1074



### Application of nucleobase-induced fluorescence enhancement in Cy3–DNA conjugates to sequence identification errors and mismatch quantification

Madhura Sohoni, Nakul Panchal and Debjani Bagchi\*

1090



### Engineering an indoleamine 2,3-dioxygenase immunotherapy *via* selective cysteine-to-serine mutations

Jennifer A. Simonovich, Arun Wanchoo, Ryan A. Clark, Junha Park, Ayumi Shigemoto, Benjamin G. Keselowsky\* and Gregory A. Hudalla\*

## RETRACTION

1099

### Retraction: Identification of MIG7, TGM2, CXCL8, and PDGFC as key genes in colon cancer with a bioinformatics-driven strategy for multi-epitope vaccine design

Zhenhai Jing, Qing Zhou, Yan Wang, Peng Meng, Yuting Duan\* and Qing Hong\*

