

# MSDE

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

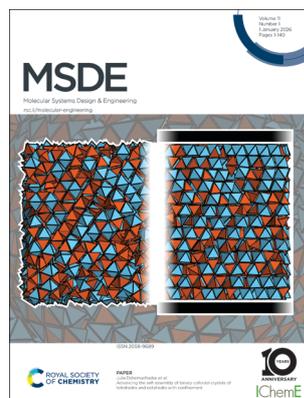
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### IN THIS ISSUE

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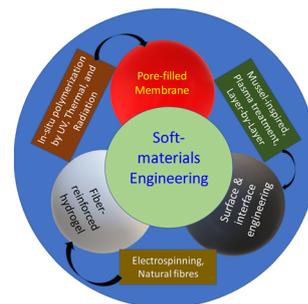
**Inside cover**  
See Julia Dshemuchadse et al., pp. 62–69.  
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### REVIEW

7

#### Soft material engineered synthetic polymer membranes: bridging design and application

Ashok K. Pandey\*

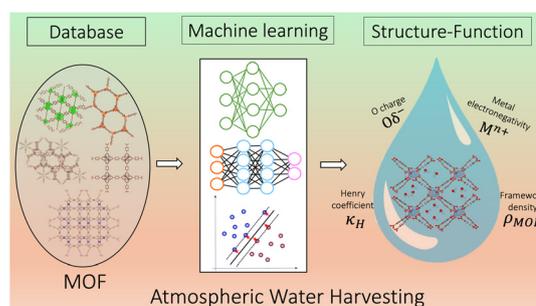


### PAPERS

50

#### Machine learning highlights chemistry as the key factor in metal-organic frameworks for atmospheric water harvesting

Nour Alkhatib, Saifeldeen Abed Alrhmam and Serdal Kirmizialtin\*





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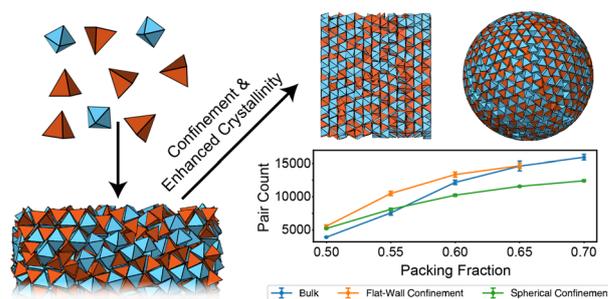
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62

## Advancing the self-assembly of binary colloidal crystals of tetrahedra and octahedra with confinement

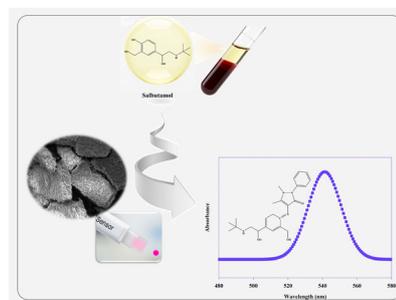
Nathan C. Huang, Rachael S. Skye and Julia Dshemuchadse\*



70

## Integrated computational and experimental design of copper-gallic acid nanozymes for selective salbutamol detection

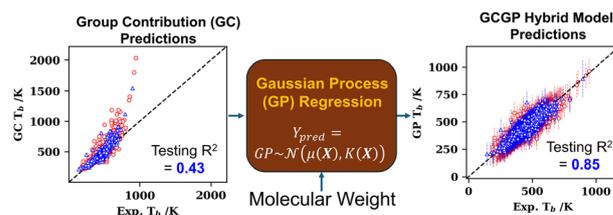
Fatemeh Parad, Fahimeh Ghasemi, Parisa Khadiv-Parsi, Haider Al Amili, Parna Keramati, Somayeh Mojtabavi\* and Mohammad Ali Faramarzi\*



85

## Enhanced thermophysical property prediction with uncertainty quantification using group contribution-Gaussian process regression

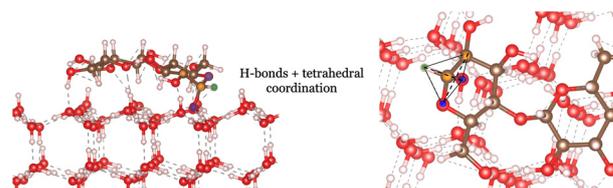
Barnabas P. Agbodekhe, Montana N. Carlozo, Dinis O. Abranches, Kyla D. Jones, Alexander W. Dowling\* and Edward J. Maginn\*



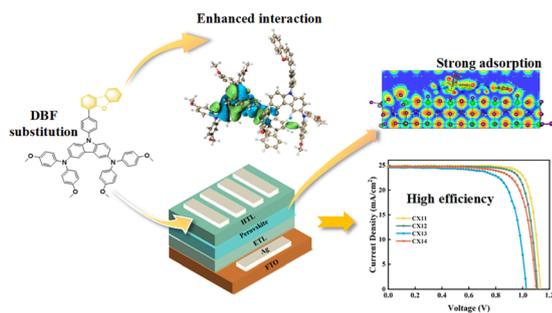
107

## A first-principles examination of the ice-cellulose interface: towards bioinspired antifreeze design

Aakash Kumar\* and Dilip Gersappe\*



118



## Strategy for the isomerization of dibenzo[*b,d*]furan-based carbazole derivatives as hole transporting materials for perovskite solar cells: theoretical design and experimental study

Xin Chen, Jiayi Qi, Xin Jiang, Fei Wu\* and Xiaorui Liu\*

126



## Simulation of the microalgae-enriched nitrogen fertilizer granulation mechanism using the DEM method

Rasa Šlinkšienė,\* Vaidas Bivainis and Austėja Mikolaitienė

