

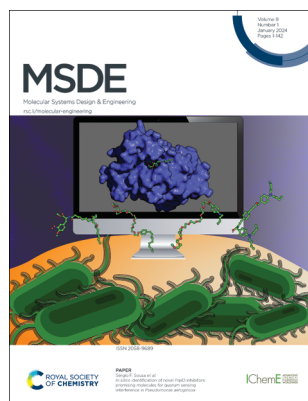
# MSDE

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

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### IN THIS ISSUE

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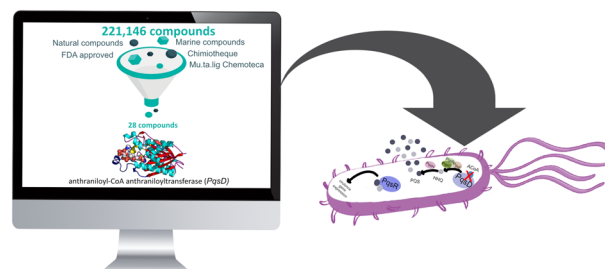
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See Sérgio F. Sousa *et al.*,  
pp. 7–19.  
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2024, 9, 7.

### PAPERS

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#### **In silico identification of novel PqsD inhibitors: promising molecules for quorum sensing interference in *Pseudomonas aeruginosa***

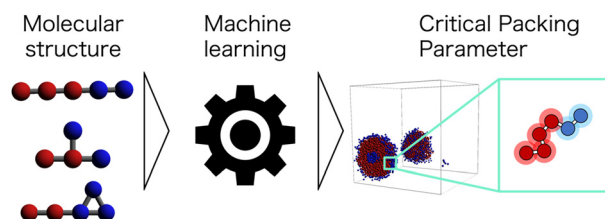
Tatiana F. Vieira, Nuno M. F. S. A. Cerqueira,  
Manuel Simões and Sérgio F. Sousa\*



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#### **Machine learning prediction of self-assembly and analysis of molecular structure dependence on the critical packing parameter**

Yuuki Ishiwatari, Takahiro Yokoyama, Tomoya Kojima,  
Taisuke Banno and Noriyoshi Arai\*





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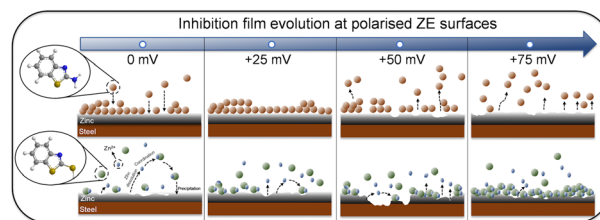
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### Inhibitory behaviour and adsorption stability of benzothiazole derivatives as corrosion inhibitors towards galvanised steel

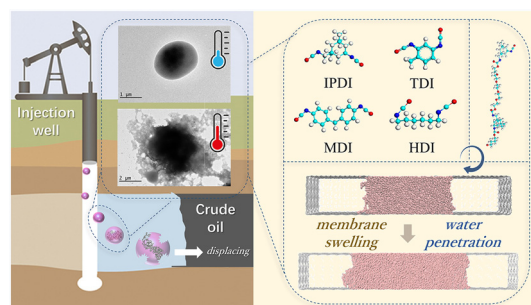
Qiushi Deng,\* José María Castillo-Robles, Ernane de Freitas Martins, Pablo Ordejón, Jan-Niclas Gorges, Philipp Eiden, Xiao-Bo Chen, Patrick Keil\* and Ivan Cole\*



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### Designing polyurethane-based microcapsules with tailored swelling behaviours for enhanced oil recovery

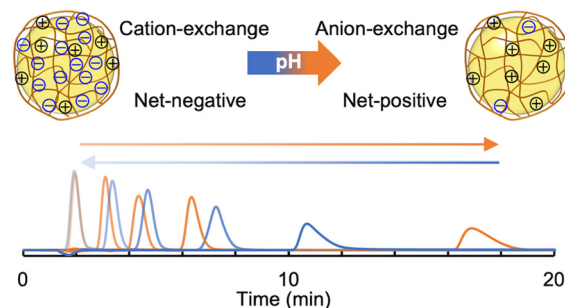
Tongyi Wang, Yongsheng Liu, Jiawei Li,\* Jun Zhang, Jian Hou, Youguo Yan\* and Xiao Wang



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### Cation/anion-exchange mode switching chromatography utilizing pH-responsive mixed charge polymer-modified silica beads

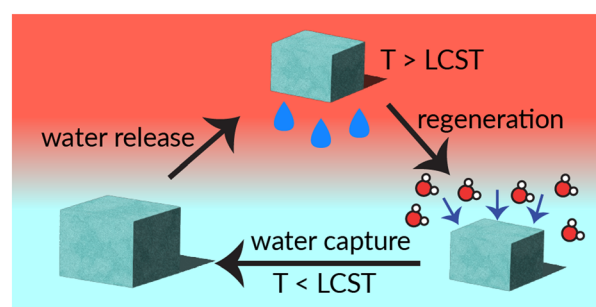
Taisei Kaku, Koichi Deura, Tomoka Yoshii, Daniel Citterio and Yuki Hiruta\*

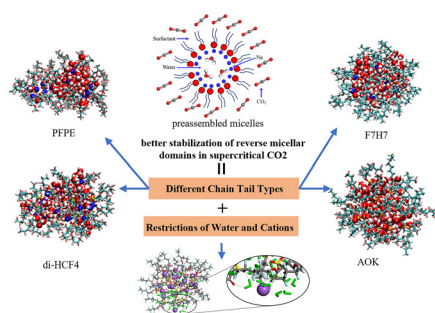


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### Rational design of water-harvesting hydrogels

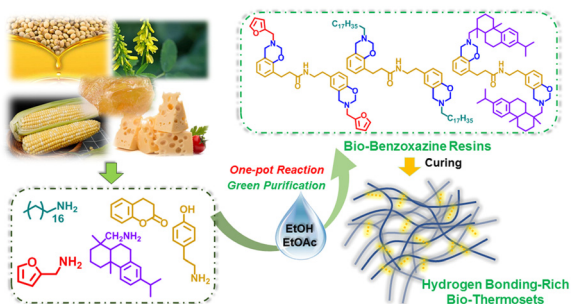
Moki K. Thanusing, Peidong Shen, Brett L. Pollard and Luke A. Connal\*





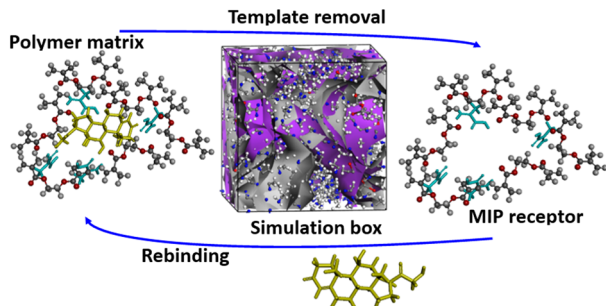
### Steric effects stabilize reverse micelle domains in supercritical CO<sub>2</sub> by determined conformation: restrictions of water and cations

Huiwen Sun, Meng Wang, Pan Wang and Muhan Wang\*



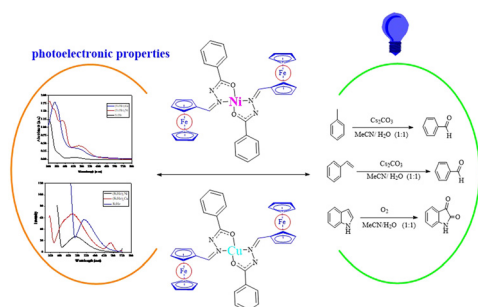
### Facile and eco-friendly synthesis of hydrogen bonding-rich bio-based bisbenzoxazine resins with low surface free energy, strong adhesion strength and high thermal stability

Yin Lu, Nan Li, Yaliang Peng, Mohamed Gamal Mohamed,\* Shiao-Wei Kuo and Kan Zhang\*



### Theoretical insights into the compatibility of template-monomer-crosslinker-solvent for cortisol molecularly imprinted polymer pre-polymerization

Victoria T. Adeleke,\* Oluwakemi Ebenezer, Madison Lasich and Samuel M. Mugo



### Bis-ferrocenyl-hydrazide metal complexes: studying electronic functional groups as newly potent homogeneous photocatalysts for C(sp<sup>3</sup>)-H and C(sp<sup>2</sup>)-H bond oxidation utilizing visible light condition

Mohammad Bashiri, Mona Hosseini-Sarvari\* and Sara Fakhraee

