

# MSDE

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

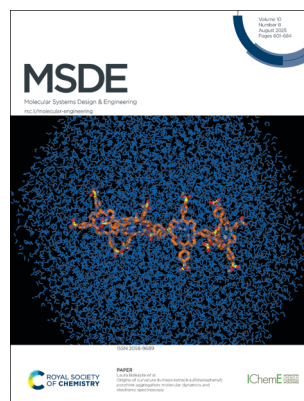
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### IN THIS ISSUE

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**Cover**  
See Gustavo Chaparro and Erich A. Müller, pp. 619–633.  
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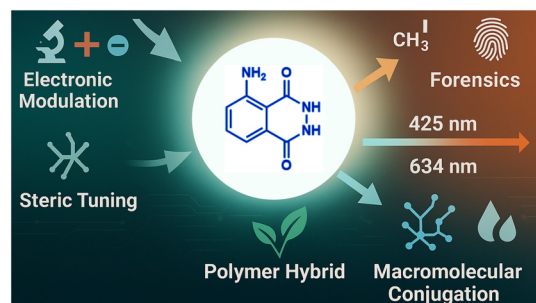
**Inside cover**  
See Laura Baliulyte et al., pp. 635–648.  
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### REVIEW

606

#### Re-engineering luminol: new frontiers in chemiluminescence chemistry

Amir M. Alsharabasy

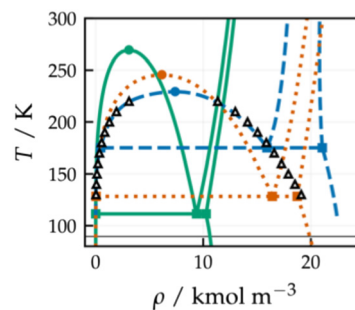


### PAPERS

620

#### Fitting a square peg in a round hole: parameterisation of quasi-spherical molecules employing the Mie potential

Gustavo Chaparro and Erich A. Müller\*



VLE  
VLE + viscosity  
VLE + solid data



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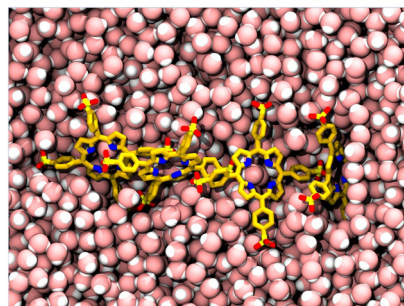
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635

### Origins of curvature in *meso*-tetra(4-sulfonatophenyl) porphine aggregation: molecular dynamics and electronic spectroscopy

Laura Baliulyte,\* Eimantas Urniezius, Vytautas Bubilaitis, Mindaugas Macernis, Lorenzo Cupellini and Darius Abramavicius



649

### Biodegradable glucosamine-amino acid-based ionic liquids as efficient water-based lubricant additives for green tribological chemistry

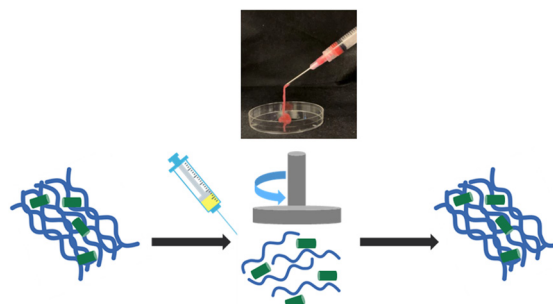
Jing Yang, Xiao Liu,\* Chongyun Sun, Qiang Chen, Pingxia Guo, Kai Feng,\* Meirong Cai\* and Feng Zhou



662

### Harnessing peptide–cellulose interactions to tailor the performance of self-assembled, injectable hydrogels

Jessica A. Thomas, Alex H. Balzer, Subhash Kalidindi and LaShanda T. J. Korley\*



675

### Flame growth of nickel-based cocatalyst for efficient solar water splitting of BiVO<sub>4</sub> photoanode

Haohua Wang, Youyi Su, Xiangui Pang, Ming Zhang, Wufang Wang, Pingping Yang, Xinxin Lu\* and Jiale Xie\*

