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Self-assembly of bis-salphen metal-organic frameworks: atomistic perspective

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The recently-observed[1] self-assembly of salphen-based metal-organic frameworks (MOF) into networks of interconnected microrings with nano-thin strings may suggests a new intriguing tool for nanoscale patterning. In particular, their ability to align very small amounts of carbon nanotubes into ultra-low density percolating network promises a breakthrough in creating highly transparent flexible thin film electrodes for illumination panels and light harvesting devices.
However, the mechanism of this phenomenon yet needs to be clarified. In this work we will show how atomistic simulations help to shed light on supramolecular structure and details of the formation of this unusual self-assembly pattern.
We use ab initio calculations and all atomic molecular dynamics simulations in explicit together with umbrella sampling and free energy perturbation to investigate conformational space of the bis-salphen MOFs and potential self-assembly pathways.
We observe that a particular conformation of the bis-salphen MOF allows it to form dimeric units, capable of linking with other units via either pi-pi or coordination Zn-O interactions in the two orthogonal directions. Due to these interactions bis-salphen MOFs can self-assemble into supramolecular chains, sheets and tubes, with highly variable mechanical properties. Furthermore, we show that the free energy gains of the two self-assembly pathways are determined by the solvent, which allows to control geometry of self-assembly and helps to relate our predictions to experimentally observed patterns.
We propose[2] that the compounds under study form a 1D coordination polymer, the fibres of which are elastic enough to fold into toroidal globules upon solvent evaporation, while being able to link separate chains into extended networks. We also explain the separate roles of atomic groups, constituting the molecule and the way solvent controls the self-assembling structure.
Intended for poster presentation.

References
[1] M.V. Escárcega-Bobadilla, G.A. Zelada-Guillén, S.V. Pyrlin, et al. Nat Commun 4, 2648 (2013).
[2] S.V. Pyrlin, N.D.M. Hine, A.W. Kleij, M.M.D. Ramos et al., Soft Matter 14(7), 1181 (2018).

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