O-I-M Seminar Series

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Hosted by Chris Hendon

Topology guided design of multivariate frameworks: Making crystals with predictable structure, variable composition, and tunable solid-state properties

Substitutional solid-solutions (SSS) are a kind of inorganic crystals that feature a constant crystal structure and a variable composition (e.g., ruby lasers [CrxAl1-x]2O3, blue LEDs InxGa1-xN). The preparation of this kind of solids is relatively easy because inorganic materials are atomic solids and form according to sphere packing models. The use of SSS strategy in molecule-based solids (organic or inorganic) is hindered by the inability to predict the crystal structure of complex non-spherical molecules. In this presentation, we show that multivariate metal-organic frameworks (MTV MOFs)—isoreticular frameworks made with mixed links—can be prepared as SSS approach by considering their underlying topology and homeomorphic relations, according to the theory of periodic nets. Targeting nets that are edge-1-transitive—those that topologically contain only one kind of edge—enabled us to prepare MTV MOFs that behave like SSS, as the mixed links compete for the same position in the crystal. We demonstrate our hypothesis by preparing MTV MOFs that exhibit complex organic-based phenomena such as molecular fluorescence (dilute, J-aggregate, multicolor, white-light, Förster resonant-energy exchange), tunable electron transfer via redox-hopping, photoredox catalysis, molecular chirality, polarity, etc., as well as MTV MOFs that follow Vegard's law. We also demonstrate how our strategy enables the preparation of MOF materials in single-crystal, thin-film, and bulk powder form for their use as applied materials with fine-tuned properties.