Polymer Program

INSTITUTE OF MATERIALS SCIENCE

Seminar: 11:10 am Friday, February 16, 2024

Science 1: Room 1002

Host: Jie He

Stephen Z. D. Cheng

Trustees Professor of Polymer Science

University of Akron

Superlattice Engineering in Giant Molecules

Abstract:: Inverse design and inverse thinking are critical steps in the new materials developments (materials genome approach). When we design materials with specific functional properties, we often start with independent building blocks ("mesoatoms") which possess well-defined molecular functions and precise chemical structures. Using the "Molecular Lego" approach, we can then, in some cases with multiple steps, assemble such elemental mesoatoms together in preferred secondary structures (or packing schemes) to construct materials possessing topologically mandated hierarchical structures with desired functions. In this talk, correlating mesoatoms with mesoscale superlattices, mimicking metal alloys, a rational engineering strategy becomes critical to generate designed periodicity with emergent properties. For molecule-based superlattices, nevertheless, nonrigid molecular features and multistep self-assembly make the molecule-to-superlattice correlation less straightforward. In addition, single component systems possess intrinsically limited volume asymmetry of self-assembled spherical mesoatoms", further hampering novel superlattices' emergence. We demonstrate that properly designed molecular systems could generate a spectrum of unconventional superlattices. We systematically explore the lattice-forming principles in unary and binary systems, unveiling how molecular stoichiometry, topology, and size differences impact the mesoatoms and further toward their superlattices. The presence of novel superlattices helps to correlate with Frank–Kasper phases previously discovered in soft matter as well as newly discovered decagonal quasi-crystals. We envision the present work offers new insights about how complex superlattices could be rationally fabricated by scalable-preparation and easy-to-process materials in their bulk states.

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