

Abstract Submitted
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Symmetry, Equivalence and Molecular Self-Organization JACK DOUGLAS, KEVIN VAN WORKUM, Polymers Division, NIST — Molecular self-organization at equilibrium is central to the formation of many biological structures and the emulation of this process through the creation of synthetic counterparts offers great promise for nanofabrication. The central problems in this field area are an understanding of how the symmetry of the interacting particles encodes the geometry of the organized structure and the nature of the thermodynamic transitions involved. Our approach is inspired by the self-organization of actin, tubulin and the icosahedral self-organization of clathrin and spherical viruses and proceeds from the general observation that biological macromolecules and synthetic molecules exhibiting supermolecular self-organization often exhibit large dipolar or other highly directional interactions, in addition to short range interactions responsible for phase separation. Correspondingly, we find chain-like, membrane-like, tubular and icosahedral particle self-organization using ‘equivalent’ particles exhibiting an interplay between directional (dipolar and multipolar) interactions and short-range (van der Waals) interactions. Specifically, a dipolar potential having a continuous rotational symmetry gives rise to chain formation while potentials having discrete rotational symmetries [e.g., square quadrupole or a triangular ring of dipoles (‘hexapole’)] led to the self-organization of sheets, hollow tubes and icosahedral structures with resemblance to biological and synthetic structures.

Jack Douglas
Polymers Division, NIST

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