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Symmetry, Equivalence and Self-Assembly

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Molecular self-assembly 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 are an understanding of how the symmetry of the interacting particles encodes the geometrical structure of the organized structure and the nature of the thermodynamic transitions involved. Our approach is inspired by the self-assembly of actin, tubulin and icosahedral structures of plant and animal viruses. We observe chain, membrane,'nanotube' and hollow icosahedron structures using 'equivalent' particles exhibiting an interplay between directional (dipolar and multi-polar) interactions and short-range (van der Waals) interactions. Specifically, a dipolar potential (continuous rotational symmetry) gives rise to chain formation, while potentials having discrete rotational symmetries (e.g., square quadrupole or triangular ring of dipoles) led to the self-organization of nanotube and icosahedral structures with some resemblance to tubulin and icosahedral viruses. The simulations are compared to theoretical models of molecular self-assembly, especially in the case of dipolar fluids where the corresponding analytic theory of equilibrium polymerization is well developed. These computations give insights into the design elements required for the development of synthetic systems exhibiting this type of organization.