Self-assembly of Ionic Chromonic Liquid Crystals

HYTHEM SIDKY, JONATHAN K. WHITMER, University of Notre Dame — Chromonic liquid crystals exhibit a unique self-assembly process which is of both theoretical and practical interest. A characteristic feature of chromonics is the occurrence of molecular association through stacking at extremely low concentrations. Experimental evidence has suggested that this process is approximately isodesmic across a broad concentration range. To date, only a handful of computational studies have managed to reproduce crucial aspects of chromonic phases, using expensive atomistic simulations. Here, we present a minimal model capable of capturing key features of the lyotropic chromonic phase. Molecular simulations of coarse-grained mesogens are used to map out the phase behavior and explore how structural and energetic anisotropies influence their ordering and response.

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