

Monte Carlo simulations of fullerite: Surface and monolayer

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In this talk, we will briefly describe the concept of plastic crystal and illustrate it with the fullerene C₆₀ crystal. We will then apply numerical techniques to solve two particular problems: The (111) crystal surface and the monolayer.

We propose a two-stage mechanism for the rotational surface disordering phase transition of fullerite. Our study uncovers the existence of a new intermediate regime, between a low temperature ordered (2×2) state, and a high temperature (1×1) disordered phase. In the intermediate regime there is partial disorder, strongest for a subset of particularly frustrated surface molecules. These concepts and calculations provide a coherent understanding of experimental observations, with possible extension to other molecular crystal surfaces.

Recently a novel rotationally ordered state was reported for fullerene monolayers physisorbed on flat neutral substrates. We show that this kind of state is an energy minimum for the standard intermolecular potential describing bulk fullerene and its surface. In the monolayer, symmetry implies a first order rotational thermal disordering.