Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Structure and properties of fullerene molecular crystals with linear-scaling van der Waals density functional theory ARASH MOSTOFI, LAMPROS ANDRINOPOULOS, Imperial College London, NICHOLAS HINE, University of Cambridge — Fullerene molecular crystals are of technological promise for their use in heterojunction photovoltaic cells. An improved theoretical understanding of their structure and properties would be a step towards the rational design of new devices. Simulations based on density-functional theory (DFT) are invaluable for developing such insight, but standard semi-local functionals do not capture the important inter-molecular van der Waals (vdW) interactions in fullerene crystals. Furthermore the computational cost associated with the large unit cells needed are at the limit or beyond the capabilities of traditional DFT methods. In this work we overcome these limitations by using our implementation of a number of vdW-DFs in the ONETEP linear-scaling DFT code to study the structural properties of C_{60} molecular crystals. Powder neutron diffraction shows that the low-temperature Pa-3 phase is orientationally ordered with individual C_{60} units rotated around the [111] direction. We fully explore the energy landscape associated with the rotation angle and find two stable structures that are energetically very close, one of which corresponds to the experimentally observed structure. We further consider the effect of orientational disorder in very large supercells of thousands of atoms.

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Date submitted: 15 Nov 2013 Electronic form version 1.4