Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Understanding the high device efficiency of a class of solution-processed small-molecule solar cells ANDRIY ZHUGAYEVYCH, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, OLENA POSTUPNA, Department of Chemistry, University of Rochester, Rochester, NY 14627, USA, SERGEI TRETIAK, Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA, GUILLERMO BAZAN, Department of Chemistry and Biochemistry, University of California, Santa Barbara, CA 93106, USA — We perform a first principles study of light absorption, exciton and charge carrier transport for two recently synthesized molecular crystals which in bulk heterojunction solar cells with PC70BM acceptor show up to 6.7% power conversion efficiency. Our results distinguish the following factors important for this high efficiency. The large conjugation length facilitates strong light absorption with low-energy absorption edge. The crystalline ordering of properly oriented molecules leads to exciton delocalization over the typical size of the crystallites. The tightly packed pi-stacks allow for fast disorder-resistant hole transport along these stacks. Nevertheless the microscopic characteristics of the considered crystals are typical and comparable with other materials used in photovoltaics. Therefore we conclude that the main factors of the high device efficiency should be searched at the mesoscale including interfaces and grain boundaries.

Andriy Zhugayevych
Theoretical Division, Los Alamos National Laboratory,
Los Alamos, NM 87545, USA

Date submitted: 27 Nov 2011 Electronic form version 1.4