Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

First principles modeling of donor materials for organic solar cells: where theory complements experiment ANDRIY ZHUGAYEVYCH, SERGEI TRETIAK, Los Alamos National Laboratory, GUILLERMO BAZAN, University of California, Santa Barbara — We discuss the predictive power and accuracy of first principles modeling of small-molecule crystalline donors for organic solar cells. First of all, in order to understand where the theory can help us in improving the performance of photovoltaic devices, we clarify what factors constituting power conversion efficiency needed to be improved. We argue these are short circuit current and fill factor, rather than bandgap and open circuit voltage. This implies that the optimization of intramolecular properties (e.g. HOMO/LUMO), which is best suitable for theoretical search, will not give the anticipated gain in efficiency. The intermolecular properties are amenable to first principles modeling on a single-crystallite scale and we discuss some challenges in this avenue. As an example of how theory can provide design rules for architecturing small-molecule crystals we analyze the dependence of charge carrier mobility on the intermolecular geometry of a pi-stack. In the other case study we show that changes in device performance due to small changes in chemical composition can be well tracked by the theory. Finally, we analyze the performance of commonly used density functionals for typical molecular systems used in organic electronics (oligomers, polymers, dimers, crystals).

Andriy Zhugayevych
Los Alamos National Laboratory

Date submitted: 07 Nov 2012 Electronic form version 1.4