Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Polaron Localization in Conjugated Polymers by Hybrid DFT Methods[1] NAN SHAO[2], QIN WU[3], Brookhaven National Laboratory, THEOREY AND COMPUTATION GROUP TEAM — Reliable application of density functional theory (DFT) to study the electronic properties of polarons remains controversial. A proper description should exhibit both the formation of a charge-localized electronic state and saturation of the polaron size for increasing oligomer length. The aim of this work is to find a proper hybrid DFT method to study the chain length related electronic properties of charged conjugated polymer system. Using oligopyrrole cations as a test case, global hybrid functionals such as BHandHLYP can show charge localization, but a well-defined polaron size does not emerge when the length of the oligomer is increased; the saturation effect was not predicted correctly. By applying 100% long-range corrected hybrid functionals, LRC-PBE, the saturation of charge distribution has been achieved, implying that the LRC-PBE is a better way to describe the spatial extent of the electronic state of polypyrrole than the conventional hybrid functionals. The tuning of the range parameter and the study of other polymer polaron systems will be discussed.

[1]Supported by Brookhaven Science Associates, LLC under Contract No. DE-AC02-98CH10886 with the U.S. Department of Energy.
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Date submitted: 09 Nov 2012 Electronic form version 1.4