Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Ab initio study of molecular packing of organic semiconducting materials SEFA DAG, LIN-WANG WANG, Lawrence Berkeley National Laboratory — The self-organizing and electronic properties of organic semiconducting material, poly(3-hexylthiophene) (P3HT), have been investigated in terms of Ab initio density functional calculations. We found that thiophene-thiophene interaction in adjacent layers has a strong influence to create stacked planar structures. Our calculations showed that P3HT chains tend to stack into planar structures, in which adjacent thiophene-thiophene rings along the stacking direction are 180^o rotated with respect to each other. Theoretical powder diffraction profile of this structure showed same structure with experimental reflection peaks. We also showed enhanced transport resulting from the organization of P3HT chains.

Sefa Dag
Lawrence Berkeley National Laboratory

Date submitted: 20 Nov 2008 Electronic form version 1.4