Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

The electronic structure and charge carrier dynamics in organic molecular crystals[1] NA SAI, The University of Texas at Austin, ZHIQIANG LI, University of California, San Diego, VITALY PODZOROV, Rutgers University, MICHAEL MARTIN, Lawrence Berkeley National Laboratory, MICHAEL GERSHENSON, Rutgers University, DIMITRI BASOV, MASSIMILIANO DI VENTRA, University of California, San Diego — Organic molecular crystal semiconductors have been receiving intense attention recently. The much higher carrier mobility and intrinsic physical properties uncovered in these materials offer many fundamental advantages over their polycrystalline counterpart. Combined with infrared absorption studies of the rubrene based field effect transistor, we study the intrinsic anisotropy in the basal a-b plane of the rubrene crystal. We report the structure and electron structure of the rubrene crystals using density-functional theory. We find fairly light effective masses of the order of the free electron mass, in agreement with those extracted from infrared measurements. In light of these results, we discuss possible mechanisms of charge transport in these crystals.

[1]Work supported by NSF.

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Date submitted: 19 Nov 2006 Electronic form version 1.4