Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

On the Charge transport regime of crystalline organic semiconductors: diffusion limited by thermal off-diagonal electronic disorder
ALESSANDRO TROISI, University of Warwick — In organic crystalline semiconductor molecular components are held together by very weak interactions and the transfer integrals between neighboring molecular orbitals are extremely sensitive to small nuclear displacements. We used a mixed quantum chemical and molecular dynamic methodology to assess the effect of thermal structural fluctuations on the modulation of the transfer integrals between close molecules. We have found that the fluctuations of the transfer integrals are of the same order of magnitude of their average value for pentacene and anthracene. This condition makes the band description inadequate because a dynamic localization takes place and the translational symmetry is completely broken for the electronic states. We also present a simple one-dimensional semiclassical model that incorporates the effects of dynamical localization and allows the numerical computation of the charge mobility for ordered organic semiconductors. These results explain several contrasting experimental observations pointing sometimes to a delocalized "band-like" transport and sometimes to the existence of strongly localized charge carriers.

Alessandro Troisi
University of Warwick

Date submitted: 30 Nov 2005 Electronic form version 1.4