

Abstract Submitted
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Role of fluctuations on electron transport in soft materials ENRIQUE GOMEZ, The Pennsylvania State University — Soft materials are characterized by weak intermolecular interactions and disorder. Although the extent of spatial fluctuations depends on the molecular structure, lattice fluctuations can be on the order of the unit cell dimensions in molecular crystals and soft materials. For example, our results from Quasi-elastic Neutron Scattering demonstrates that longer side chains in poly(3-alkylthiophene)s leads to an enhancement in motion of the thiophene rings. To ascertain the effect of dynamics on charge transport, we have developed a simple model to describe the roles of longitudinal and transverse modes of the intermolecular spacing between molecules on intrinsic electron mobilities. We demonstrate that the intrinsic mobility of soft materials appears thermally-activated by assuming fluctuations in a harmonic potential and an exponential decay in the charge transfer rate with intermolecular distance. For example, for poly(3-hexylthiophene), we can extract the characteristic decay as a function of separation distance from Density Functional Theory calculations and the extent of fluctuations from Molecular Dynamics simulations to predict the temperature dependence of the charge mobility. We find that the temperature dependence appears Arrhenius with activation energy of approximately 50 meV for a wide temperature range, in good agreement with experiments. This model suggests that fluctuations in the lattice spacing of soft materials lead to a significant intrinsic dependence of electron transport on temperature, regardless of the presence of band-tail states or traps.

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