

Abstract Submitted
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Computational Simulation of Charge Transport in Metal Terpyridine Monolayer FETs MARCUS HANWELL, GEOFFREY HUTCHISON, University of Pittsburgh — Understanding the roles of charge traps and defects in electronic transport in organic materials is becoming increasingly important. Computational studies have been undertaken, using an agent-based Monte Carlo method, of the active region of a monolayer FET. Charge transport is assumed to be due to thermally activated, variable-range hopping between neighboring sites. This model system allows us to probe the role of charge traps/defects both computationally and experimentally. We do this by using multiple metal terpyridine complexes, each having known electronic structure. Using Marcus Theory and quantum calculations, the hopping rate between neighboring complexes can be predicted. Results from computational simulations of this system will be discussed, with special attention being paid to the results that can be experimentally verified, such as voltage-current curves.

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