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Monte Carlo modeling of charge transport in nanocrystalline PbSe films IAN CARBONE, University of California, Santa Cruz, GERGELY ZIMANYI, University of California, Davis, SUE CARTER, University of California, Santa Cruz — The electronic properties of three-dimensional nanocrystalline (NC) PbSe materials are of particular interest for next generation solar energy conversion technologies. With size-tunable optical and electronic properties, solution processing, and multiple exciton generation, these materials could represent an exciting new class of cost-effective and efficient solar cells. Two models, a multiple trapping random walk(MTRW) and a hopping model, were developed to simulate electron and hole transport in films of PbSe nanoparticles crosslinked with ethane dithiol ligands. This Monte Carlo code could easily be adapted to model solar cell current-voltage characteristics and variety of experimental conditions and device structures. In both simulations, films are represented by a regular cubic lattice, transport is carried out as a series of hopping events between neighboring nanocrystals, and electrons occupy energetic states determined by the particle size of the PbSe nanocrystals. We find that the hopping model represents a simpler parameter set and a better match to experimental measurements. This presentation will discuss the two transport mechanisms and the effects of particle size, energetic disorder, and coulomb blockade effects on electron and hole mobilities.

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