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Equilibrium Charge Transport in Nanocrystal Solids: Polaron Effects

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Abstract. Nanocrystal solids, also known as colloidal quantum dot supercrystals, are novel type of structures with colloidal quantum dots self-arranged into a lattice. It was suggested that these artificial solids may exhibit band-like transport paving the way for new cheap optoelectronic technologies [1]. However, it seems that many physical effects are preventing band-like transport such as disorder, weak electronic coupling of adjacent dots, dielectric response of ligand matrix and electron-phonon interaction [2]. We studied the effects of electron-phonon interaction on transport properties of these structures. We have modeled these structures using the generalization of the Holstein model with multiple localized phonon modes per each site/dot. Phonon energies and electron-phonon coupling constants were obtained by employing the elastic and dielectric continuum models. The model was then analyzed using a variational approach which gives exact solutions in two limiting cases, strong electron-phonon coupling regime and weak electron-phonon coupling regime. By minimizing the upper bound of free energy, we have identified that recently fabricated structures are in strong coupling regime. Using linear response theory we calculated the mobility of carriers and identified the small polaron hopping nature of transport. Even though mobility decreases by increasing the temperature, we show that band-like transport is still not achieved in these structures [3].

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