Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Metal-Insulator Transition in nanoparticle solids: a kinetic Monte Carlo study[1] GERGELY ZIMANYI, LUMAN QU, Physics, UC Davis, Davis, CA 95616, MARTON VOROS, Materials Science Division, Argonne National Laboratory, IL — Nanoparticle (NP) solids recently emerged as a promising platform for high performance electronic/optoelectronic devices, including third generation solar cells, light emitting diodes and field effect transistors. A challenge of NP films is that their charge transport is in the unfavorable hopping/insulating regime. Recent experiments showed that it is possible to tune the NP solids through a Metal-Insulator Transition (MIT) via ligand engineering and ALD matrix infilling. However, the microscopic understanding of this transition is not yet clear. To address this challenge, we developed a Kinetic Monte Carlo transport modeling framework that builds on determining NP parameters from ab initio-based calculations of the energy level structures, charging energies and overlaps, and then uses these to compute the hopping mobility across a disordered NP array by the Marcus and Miller-Abrahams mechanisms. We reproduced and explained the observed non-monotonous dependence of the mobility on the NP diameter. Centrally, we extended our platform to be able to capture the MIT. We determined the MIT phase boundary on the (NP-NP overlap - Electron density) plane. We demonstrated that all mobilities fall on a universal scaling curve, allowing us to determine the critical behavior across the MIT.

[1]Supported by: UC Davis Office of Research RISE ANSWER grant

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Date submitted: 06 Nov 2015 Electronic form version 1.4