Studies of Thermal Conductivity in Hybrid Organic-Inorganic Nanocrystal Arrays

WEE-LIAT ONG, Carnegie Mellon University, SARA RUPICH, DMITRI TALAPIN, University of Chicago, ALAN MCGAUGHEY, JONATHAN MALEN, Carnegie Mellon University — The thermal conductivity of nanocrystal arrays (NCAs) is studied and found to be tunable through the nanocrystal diameter, and chemistry - a conclusion that is supported by our Molecular Dynamics simulation. Nanocrystal arrays self-assemble from colloidal molecule-coated nanocrystals into close-packed 3D films. It has been suggested that their electronic and thermal transport properties can be decoupled, enabling a resolution to the conflicting needs of various thermal management and solid-state energy conversion applications (e.g. high figures of merit materials for thermoelectric, high-efficiency photovoltaic materials). Although the electronic transport in NCAs has been studied extensively, little is known about their thermal transport. We herein report both experimental measurements and modeling performed to elucidate the thermal transport mechanisms in NCAs. Various factors including the geometry and chemical compositions of the NCAs will be presented. Simulation results showed good agreement with the observed experimental trends, providing a complementary computational approach for elucidating and optimizing NCA thermal properties.