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Probing tunable thermal properties of organic hetero-junctions SHUBHADITYA MAJUMDAR, SCOTT N. SCHIFFRES, JONATHAN A. MALEN, ALAN J.H. MCGAUGHEY, Carnegie Mellon University — The ability to tune physical properties of new organic-inorganic heterojunctions is essential for their popularity in the fields of molecular electronics and energy-generation devices. Intimate associations between the organic and inorganic components at the nanoscale level lead these materials to possess unique transport properties. Here, we probe the thermal conductance of self-assembled monolayer (SAM) junctions using both computational and experimental methods. SAM junctions are ordered, periodic arrays of a single layer of organic molecules chemically bonded to two inorganic substrates. Molecular dynamics simulations are performed on the SAM junctions to study the effect of physical parameters on the junction thermal conductance. These include atomic masses of leads, junction temperature, molecular chain length, and surface coverage. Another important aspect is the contribution of the stiff C-H bonds to thermal transport, an analysis of which is also presented. Lattice dynamics calculations are employed to study the effect of molecular vibrations on the thermal coupling between the leads. The SAM junctions are prepared in the laboratory through a combination of solution immersion and transfer printing techniques. Frequency domain thermo-reflectance (FDTR) – a laser-based non-contact measurement scheme to probe the thermal properties of thin films, is employed to study the samples. A comparison between the results obtained from these studies is thus presented.

Shubhaditya Majumdar
Carnegie Mellon University

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