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The role of molecular layer mixing on the thermal conductance of organic-inorganic heterojunctions SHUBHADITYA MAJUMDAR, ALAN J.H. MCGAUGHEY, JONATHAN A. MALEN, Carnegie Mellon University — The role of interfacial properties in affecting energy transport characteristics is an extensive area of research. Hybrid materials composed of organic-inorganic heterojunctions are gaining popularity as alternatives to conventional semiconductors for various energy-generation devices, thus requiring detailed study of their interfacial properties – especially thermal transport. Previous works have isolated the organic-inorganic interface thermal properties using self-assembled monolayer (SAM) junctions between two inorganic substrates and characterized them based on interfacial bonding strength, vibrational mismatch and molecule length. Here, we investigate the effect of having a mixed SAM layer on the thermal conductance of the SAM junction. The mixed SAM layers either have molecules of the same length but different end groups (thiols and methyl) or different lengths. This creates a modifiable bonding environment at one interface either through a varying ratio of strong and weakly bonded end groups or a decreasing surface coverage of the molecule. Both these scenarios are investigated to study the cooperative nature of the molecules/interface bonds and their effect on the heat transport across the junction. We follow a combined experimental and computational approach in our investigation – we fabricate the SAM junctions (alkanethiols between two gold substrates) and measure their thermal conductance using Frequency Domain Thermoreflectance, and use molecular dynamics simulations to get a deeper understanding of the role of intermolecular cross talk.

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