Interfacial Thermal Conductance of Thiolate-Protected Gold Surfaces <u>Suzanne M. Neidhart</u>, J.D. Gezelter¹ University of Notre Dame ¹251 Nieuwland Science Hall, Notre Dame, Indiana, 46556, United States

Molecular dynamics simulations of thiolate-protected and solvated gold nanoparticles and planar surfaces were carried out in the presence of a non-equilibrium heat flux between the solvent and the core of the particle. The interfacial thermal conductance (G) was computed for these interfaces, and the behavior of the thermal conductance was studied as a function of particle size, ligand flexibility, and ligand chain length. In all cases, thermal conductance of the ligand-protected particles was higher than the bare metal–solvent interface. A number of mechanisms for the enhanced conductance were investigated, including thiolate-driven corrugation of the metal surface, solvent ordering at the interface, solvent-ligand interpenetration, and ligand ordering relative to the particle surface. Only the smallest particles exhibited significant corrugation. All ligands permitted substantial solvent-ligand interpenetration, and ligand chain length has a significant influence on the orientational ordering of interfacial solvent. Solvent – ligand vibrational overlap, particularly in the low frequency range (< 80cm⁻¹) was significantly altered by ligand rigidity, and had direct influence on the interfacial thermal conductance.