The Role of Surface Functionalization in Thermal Transport across Hard-Soft Material Interfaces

T. Luo[1]

[1] *Aerospace and Mechanical Engineering, University of Notre Dame, Notre Dame, USA*

Thermal transport across interfaces between hard and soft materials are of both scientific and technological importance. These interfaces are seen in composite materials, electronics packaging, biomedical applications and etc. In this talk, I will discuss a series of molecular simulations of the thermal transport physics across hard-soft interfaces. I will discuss the interplay between the interfacial bonding effect, the vibration coupling effect, and interfacial molecular structural effect with the overall thermal conductance. The results demonstrate that unconventional thermal transport enhancement can be achieved by properly functionalizing the hard surface with small ligands. Despite the fact that the ligands weaken the interfacial bonding between the hard and soft materials, the thermal conductance can be significantly enhanced. Such counter-intuitive enhancement is the result from the special functional ligands, which bridge the vibrational spectra mismatch between the hard and soft materials. Such a strategy can be combined with the interfacial bonding effect to further enhance the thermal transport. I will show that by further promoting hydrogen bonds between the functional ligands and the soft material, the interfacial thermal conductance is further improved. Molecular simulations show that the enhancement is not only due to stronger hydrogen bonds, but also the interfacial molecular structural change induced by them.

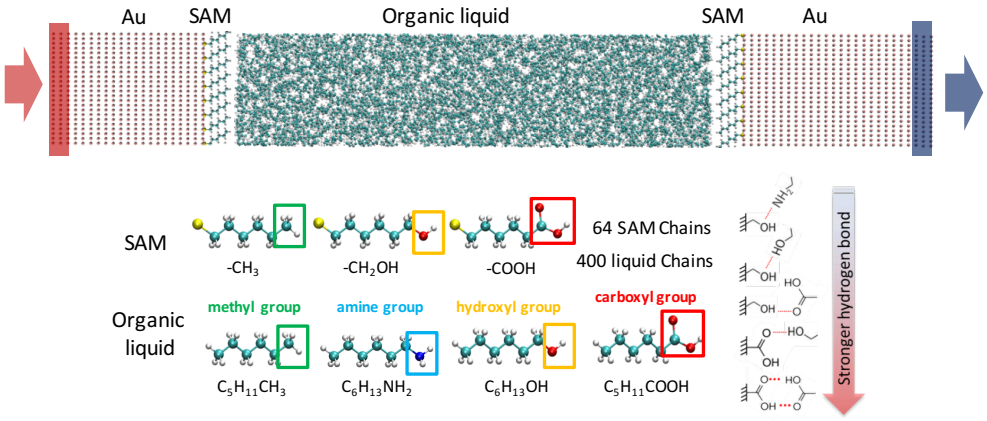

Fig. 1: Thermal transport across hard-soft material interfaces.