Bulk nanomaterials and nanoscopically-tailored heterointerfaces for heat management, power harvesting and electronics

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The first part of my talk will describe new molecularly-directed approaches to scalably create novel bulk nanomaterials through directed synthesis and assembly for a wide variety of applications. I will demonstrate the realization of a new class of high-figure-of-merit bulk nanothermoelectrics for transformative refrigeration and power harvesting technologies. The nanobulk pnictogen chalcogenides, obtained by the assembly of doped nanocrystals synthesized by a microwave-stimulated surfactant-mediated solvothermal route, exhibit 25-250% higher figure of merit than their non-nanostructured bulk counterparts. A combination of nanostructuring, sulfur doping and alloying yields ultralow lattice thermal conductivities together with electrical conductivities and high Seebeck coefficients, with control over the majority carrier type. I will discuss the property enhancement mechanisms based on electron microscopy and spectroscopy, and measurements on individual nanostructures and their assemblies. I will also demonstrate the transmutability of our approach to Al-doped ZnO, nanocomposites to obtain twenty-fold lower lattice thermal conductivity than non-nanostructured ZnO while retaining bulk-like power factor, leading to 50% higher figure of merit at 1000 K.

The second part of my talk will describe new approaches to understand and molecularly manipulate the chemo-mechanical integrity and thermal transport properties of heterointerfaces germane to applications such as nanoelectronics, lighting, energy generation and nanocomposites. I will show that introducing an organic nanomolecular monolayer at a metal-dielectric interface can lead to factorial increases in interfacial fracture toughness. I will show that this concept can be harnessed to facilitate the adhesion of inherently non-adherent materials, and to tune and obtain three- to four-fold increase in the thermal conductance of Cu-silica interfaces through the use of adhesion-enhancing moieties. Molecular dynamics simulation and a vibrational analysis of the nanomolecularly tailored interfaces indicate that thermal conductance enhancement is enabled by overlaps in low-frequency vibrational states across the interface. These unexpected results are contrary to the prevalent notion that soft organic materials are not appropriate for facilitating thermal transport, and pave the way for rational control of interfacial thermal conductivity. I will also show the use of magnetic nanofluids to tune the interfacial thermal conductivity for larger scale systems.

I will conclude my talk with an example of how nanomolecular functionalization can be used to access nanoscale processes such as the atomic-scale mechanics of heterointerfacial fracture.

Selected relevant references