

A new class of bulk thermoelectric nanomaterials from nanocrystals sculpted by molecularly-directed synthesis and doping

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This talk will describe a new strategy to realize bulk nanomaterials with control over multiple properties through the use of a molecularly-directed synthesis approach that combines nanostructuring and doping. I will demonstrate a new class of doped-nanothermoelectrics obtained by the assembly of surfactant-sculpted nanocrystals synthesized by a scalable microwave-solvothermal approach. I will show that besides providing the means to shape, size and protect the nanocrystals, the surfactant serves as a doping agent, thereby allowing the manipulation of electronic and thermoelectric properties. Sintered nanostructure assemblies exhibit up to 250% higher figure of merit than their non-nanostructured non-alloyed counterparts. While nanostructuring leads to ultralow thermal conductivities, sub- to few-atomic-percent doping retains high charge carrier mobilities and allows efficient control over carrier concentration and type through alterations in defect chemistry and electronic band structure, leading to high electrical conductivities and high Seebeck coefficients. Manipulating structures at different length-scales is thus attractive to untangle unfavorably correlated properties. I will briefly show that similar effects can be obtained through control of multiple dopants. Atomistic and electronic mechanisms of property control and enhancement will be discussed based upon electron microscopy, spectroscopy and density functional theory calculations for sulfur-doped V-VI compounds and Al-/Bi-doped ZnO. Our findings open up transformative solid-state refrigeration and waste-heat harvesting technologies, and may be transmuted for creating multifunctional materials for other applications.

References

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