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Computational design for low-temperature thermoelectric materials

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Thermoelectric materials are usually doped with external impurity atoms which provide the required level of carrier concentration (electrons/holes) for a good electronic performance. These impurity atoms scatter the conduction carriers and limit their mobility. Such limitation can be improved by introducing new doping schemes. For instance, impurity atoms can be substituted by metallic/ semi-metallic nanoparticles, or heavily doped semiconducting grains/nanowires can be embedded inside a host matrix in order to create a three dimensional modulation doping structure. We have recently demonstrated three dimensional modulation doping scheme in nanostructured SiGe materials and observed about 40% enhancement in the carrier mobility compared to uniform doping. The enhancement could be much larger if a complete separation of carriers and ions is achieved e.g. by addition of a spacer layer It is possible to shield the nanoparticles with a coating layer to minimize the conduction carrier scattering and reduce the scattering cross section by 4 orders of magnitudes below the physical cross section to cloak the nanoclusters and to design invisible dopants. Extension of such a design to realistic materials can increase the carrier mobility by orders of magnitude especially at low temperatures, and can potentially increase the thermoelectric performance by two orders of magnitude.