Electronic Structure Calculations of Thermoelectric Materials and Semiconductor Nanowires

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Electronic structure calculations have played a more and more important role in understanding materials properties, explaining experimental observations, and designing new functional systems. In this talk, I will present my recent work based on electronic structure calculations by using first-principle density functional and empirical atomic pseudopotential methods. These are involved with two specific topics: (i) transport properties of thermoelectric materials (ii) electronic and excitonic properties of semiconductor nanowires. Thermoelectrics for waste heat recovery is the subject of considerable recent interest that derives from efforts to improve energy efficiency and reduce CO$_2$ emissions. Here I will discuss several interesting material systems toward potential new thermoelectrics. Semiconductor nanowires have attracted a lot of attention as the promising candidate for application in such as electron, thermoelectrics, photonics, and photovoltaic devices. In this part I will show a number of exotic electronic changes occurring in quantum nanowires induced by quantum confinement. These predictions will be helpful to explain experiments and design devices.