Density functional theory study of the electronic structure and transport properties of La, V, Nb, and Ta doped $SrTiO_3$

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研究目的: First-principles calculation of crystal structure, electronic structure and thermoelectric properties in donor doped $SrTiO_3$ have been studied in presence of spin-orbit coupling (all calculations used PCC)

研究内容の概要: Enhancing the electronic transport properties of SrTiO3 (STO) through tuning the electronic structure by dopant substitution is of great interest in view of potential application of STO to thermoelectric energy harvesting devices. A large power factor has been reported for La, Nb and oxygen vacancy doped STO, generating significant interest in theoretical approaches to predict the magnitude, carrier concentration, and temperature dependence of the Seebeck coefficient. In this research, the electronic transport properties of donor doped STO was theoretically studied by first principles calculations including the spin-orbit (SO) interaction and low field Boltzmann transport theory, for pure STO and STO doped with La, V, Nb, and Ta.

結果: The dopant induced changes to the electronic structure, band masses, density-of states masses, split-off energies, and transport properties were systematically studied and the degree to which the calculated Seebeck coefficient (S) predicts the magnitude of the experimental Seebeck data was explored. We have found that, while SO coupling significantly decreases the band masses along the Γ-X direction, the calculated density-of-states masses exhibit a significantly smaller variation for all studied systems, with Seebeck coefficients in the range of -21.39 μV/K to -41.30 μV/K for 1 dopant per 2x2x2 STO supercell. At lower carrier concentrations and temperatures, the SO coupling has a marked effect on both the filling dependence of the density-of-states mass as well as on the temperature dependence of the Seebeck coefficient, with quantitative theoretical predictions of the temperature dependence of S in closer agreement to experimental data than those based on DFT calculations that do not include the SO interaction.

Electronic structure of Nb-doped STO