First Principles Study on Thermal Transport in Perovskite Oxides

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Perovskite oxides with ABO3 structures are promising candidates to be used as transparent conducting oxide in optoelectronic devices and as the channel material in high mobility oxide electronics. In this work, we calculate the lattice thermal conductivity of several perovskite oxides by solving the phonon Boltzmann transport equations with interatomic force constants from first principles calculations. We compare the phonon transport characteristics in different oxides and illustrate the mechanisms that determine their thermal conductivity. We also investigate the effects of oxygen vacancy, impurity, and lattice strain on the phonon transport and thermal conductivity. In $BaSnO_3$, we find the reduction of thermal conductivity at 300 K due to oxygen vacancies are mainly caused by the increased scattering of those low-frequency optical phonons. The lanthanum and antimony impurities have little effect on the thermal conductivity, but the potassium impurity significantly lowers the thermal conductivity by increasing the scattering rate of dominant phonons including both the acoustic modes and the low frequency optical modes. By applying an isotropic tensile strain of 2 %, the thermal conductivity at 300 K is decreased by 45 %, which can be attributed to the decrease of phonon group velocity, the decrease of heat capacity of dominant phonons, and the increase of phase space for three-phonon scattering. The findings in this study will help us to understand the mechanisms of thermal transport in perovskite oxides and provide guidelines for engineering their thermal properties while taking into consideration the impurity, vacancy, and strain.