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Thermal Transport Properties of Single-Layer Gray-Arsenic

Using various theoretical methods, we investigate the thermoelectric property of gray arsenic. Thermoelectric devices that utilize the Seebeck effect convert heat flow into electrical energy. The conversion efficiency of such a device is determined by its figure of merit or ZT value, which is related to various transport coefficients, such as Seebeck coefficient and the ratio of its electrical conductivity to its thermal counterpart for given temperature. To calculate various transport coefficients and thus the ZT values of gray arsenic, we apply the Boltzmann transport theory to its electronic and phononic structures obtained by density functional theory and density functional perturbation theory together with maximally localized Wannier functions. During this procedure, we evaluate its relaxation time accurately by explicitlyconsidering electron-phonon coupling.

Figures

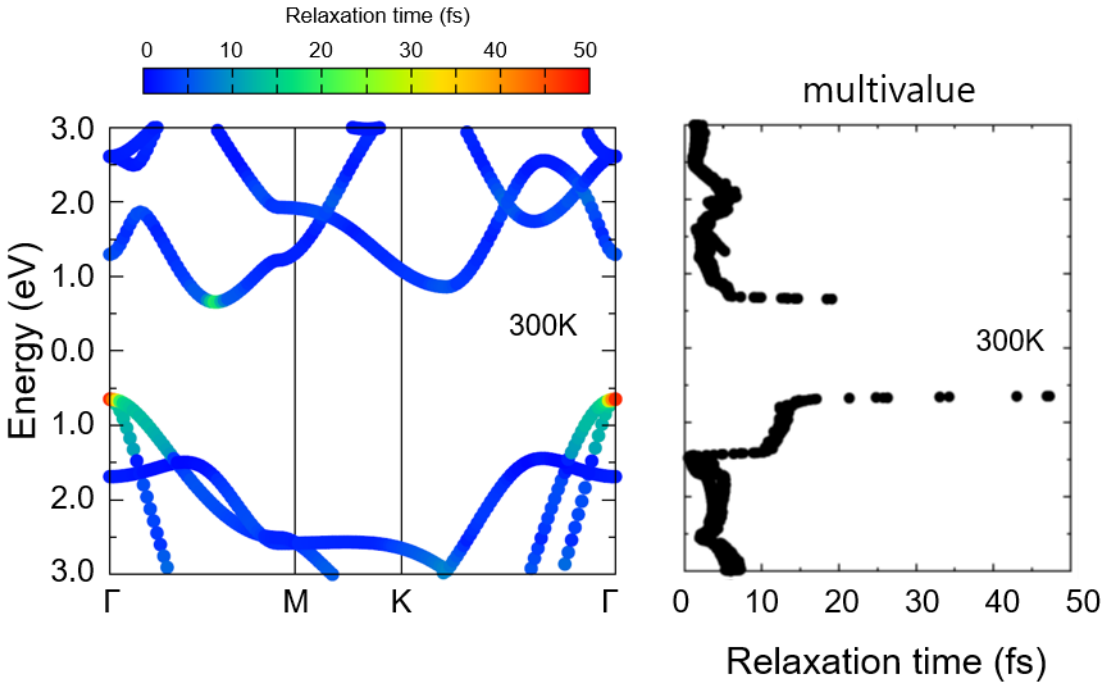

Figure 1: The color-coded band structure for the relaxation time at the Room temperatura. Although the main contribution of relaxation time is at the band edges, the other k also contributes to relaxation time. In the full BZ, relaxation time is multivalued at each energy.