Electron-phonon interactions from first-principles in bulk- and device structures

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The interaction between electrons and phonons plays an important role for the transport properties of both bulk- and device-like systems. The room-temperature mobility of industrially relevant semiconductors is typically limited by electron-phonon scattering, thus reducing the electronic current. On the other hand, in certain device-systems, the electron-phonon interaction can lead to a pronounced increase in current. This is true for pn-junction and tunnel field effect transistors (TFETs) in the off-state. In certain molecular junctions, the current can also increase by orders of magnitude due to the electron-phonon interaction, and the same is true for electron transport across certain grain boundaries. In this presentation, we will show our recent development in implementing electron-phonon interactions in ATK for studying both bulk and device systems exemplified with the above-mentioned cases.

The image below shows the effect of inelastic tunnel currents in a p-n junction.