Wannier interpolation study of the Elliot-Yafet spin relaxation in metals
ERIC ROMAN, IVO SOUZA, University of California, Berkeley, JONATHAN YATES, Cambridge University, United Kingdom — Energy states of nonmagnetic metals may be chosen to be purely spin up and down in the absence of spin-orbit coupling. Spin-orbit coupling mixes the two states by a small amount $b^2$. A spin-conserving interaction (e.g. electron-phonon) causes transitions between the two states, and flips the electron’s spin. Some insight into this Elliot-Yafet spin relaxation mechanism can be obtained by averaging $b^2$ over the Fermi surface. In trivalent metals, such as aluminum, $b^2 \ll 1$ almost everywhere on the Fermi surface, except at small “hot spot” regions. $^1$ Although the small regions of large $b^2$ dominate the spin relaxation process, they are difficult to capture numerically. We describe a Wannier interpolation strategy $^2$ to compute $\langle b^2 \rangle$. We validate it by performing ab initio calculations on aluminum, finding good agreement with previous results.$^1$ We also discuss interpolating ab initio electron-phonon matrix elements to compute the spin relaxation rate.