

O.34 Phonon-limited conductivity in 2D and 3D metals

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Computing the carriers lifetime and conductivity of metals requires a fine q-point sampling of the Fermi surface. In this project, we test the capabilities of Abinit to achieve an efficient q-point sampling to compute the conductivity within the self-energy relaxation time approximation. At a temperature high enough for the conductivity to be limited by phonon, the electrical conductivity of bulk 3D copper calculated with Abinit is in good agreement with the experimental value. We study MXenes, a class of two-dimensional inorganic compounds with interesting and complex electrical properties, namely 2D $Ti_3C_2(OH)_2$ and the 2D $Ti_3C_2F_2$. We will present results of the electrical conductivity with respect to different k-point and q-point grid.