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Interplay between Superconductivity and Strain in Al and Nb from First-Principles: a Maximally Localized Wannier Functions Approach M. SALVETTI, N. BONINI, D. PARKS, N. MARZARI, MIT, M. CALANDRA, Institut de Minéralogie et de Physique des Milieux Condensés — Phonon-mediated *el-el* interactions are the microscopic basis of low temperature superconductivity. The Eliashberg-Migdal theory formulates the problem in terms of *el-ph* matrix elements and corresponding *el-ph* linewidths. In principle, *ab-initio* DFT codes based on pseudo-potentials and plane-waves can provide an accurate prediction of the *el-ph* linewidth spectrum over the entire Brillouin zone in bulk materials. In practice, fully converged calculations are often unattainable because of the required dense samplings of the Fermi surfaces and limitations in the available CPU time. In many cases, the reformulation of the *el-ph* matrix problem using maximally localized Wannier functions reduces the time-consuming part of the calculation to the determination of the phonon frequencies via linear perturbation DFT and leads to a fully-physical based interpolation technique. Here, we present results on the superconducting critical temperature T_c of Al and Nb crystals under various mechanically-strained configurations and show that even in such simple bulk systems the use of the Wannier basis approach is necessary to ensure accurate and reasonably fast calculations.

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