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Superconductivity in lithium under pressure from electron-phonon coupling¹ TIMUR BAZHIROV, JESSE NOFFSINGER, MARVIN COHEN, Department of Physics, University of California, Berkeley; Material Science Division, Lawrence Berkeley National Laboratory — Lithium exhibits a very high superconducting transition temperature at pressures above 20 GPa. To explore the role of phonon induced pairing of the electrons, we apply first principle techniques based on the pseudopotential density functional approach and the Wannier interpolation method to calculate the electron-phonon coupling properties of lithium for the pressure range of 10-40 GPa. We are able to sample a very fine k-point grid with up to several million points in the Brillouin zone (BZ). The Fermi surface (FS) nesting features and phonon renormalizations were examined. Our results for the coupling strengths and phonon linewidths are consistent with previous studies where high resolution was not yet available. The pressure increase results in an increase in the electron-phonon coupling parameter throughout the BZ. We find that the pressure dependent coupling is also related to the shape of the FS. The calculated Tc is in agreement with experiment.

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