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First-Principles Investigation of Superconductivity in Transition Metal Carbides[1] JESSE NOFFSINGER, FELICIANO GIUSTINO, STEVEN G. LOUIE, MARVIN L. COHEN, UC Berkeley, Lawrence Berkeley National Laboratory — We investigate the origin of superconductivity in the transition metal carbides TaC and HfC by a first-principles approach. The electronic structure is described within density functional theory in the local density approximation, and the lattice dynamical properties are determined through density functional perturbation theory. We calculate the average electron-phonon coupling strength through the isotropic approximation to the Migdal-Eliashberg theory, and the superconducting transition temperature through the McMillan formula. The calculated transition temperatures are found to be in excellent agreement with experiment. The relatively high transition temperature of TaC (10.3 K) is associated with a Kohn anomaly in the phonon dispersions, and arises from significant Fermi surface nesting. In contrast, the absence of nesting in HfC results in a limited phase-space availability for electron-phonon scattering. Correspondingly, HfC exhibits a negligible transition temperature (< 0.1 K).

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