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Origin of large electron-phonon coupling in the metallic hydride TiH_2[1] SHANAVAS K. VEEDU, DAVID S. PARKER, Oak Ridge National Laboratory — The recent discovery of large superconducting transition temperature of $T_c = 190$ K in metallic H_2S under high pressures of 200 GPa, has renewed the interest in the superconducting properties of metal-hydrogen systems. These materials are expected to be electron-phonon superconductors and hydrogen with its low mass can contribute new optic phonons that may couple with the conduction electrons. Often, though not always, a large electron-phonon coupling parameter λ (and consequently high T_c) can result from a high electronic density of states at the Fermi level ($N(E_F)$) and the presence of soft phonons. With the help of first-principles calculations within density functional theory, we studied the cubic TiH_2 which has a large $3d$ $N(E_F) = 2.8$ states/eV/f.u. Our calculated phonon dispersions show that Ti modes active below frequencies of 10 THz whereas much lighter H modes are active between 32 and 40 THz. Electron-phonon coupling calculations reveal a $\lambda = 0.98$ which corresponds to a $T_c = 6.1$ K. However, the large $N(E_F)$ also leads to a tetragonal instability at low temperatures in TiH_2, which may be overcome by a uniaxial strain, potentially making it a candidate for electron-phonon superconductor.

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