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Influence of Fermi Surface Topology on Superconductivity in High-Pressure Phases of Silane[1] TIAN CUI, XILIAN JIN, State Key Lab of Superhard Materials, Jilin University — Both a semimetallic molecular phase with $P2_1/m$ symmetry and a metallic atomic phase with $P2_1/c$ symmetry are found using *ab initio* geometry optimization method from initial configurations of random molecular SiH_4 and atoms Si and H, respectively. The molecular phase shows a pressure-induced metallization, which can be described quantitatively by Fermi surface (FS) filling constant defined in our work. The lower superconducting critical temperature (Tc) about 16.2 K at 175 GPa and its peculiar superconductive behavior that its Tc decreases initially and increases later with pressure agree with a recent experimental results. Different electron-phonon coupling mechanisms are uncovered during the increase and decrease of Tc with pressure. The atomic phase shows a higher Tc of about 47 K at 190GPa and its Tc increases with pressure in its dynamically stable range. The FS filling constant and FS topology transitions under pressure mostly account for the different superconductivity between the molecular and atomic phases.

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