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The effect of pressure and doping on SrPt₃P superconductor: First-principles calculations. ARMINDO S. CUAMBA, HONG-YAN LU, CHIN S. TING, Univ of Houston, ARMINDO S. CUAMBA, HONG-YAN LU, C.S. TING TEAM — Recently, experiments of resistivity and magnetization on SrPt₃P under pressure and doping have been conducted by B. Jawdat et al., (Phys.RevB.91,094514(2015)), it was found that with the increase of pressure, the superconducting transition temperature T_c first increases with the maximal at 0.99 Gpa and then decreases, while the Si doping suppress T_c. In this work, we investigate the electronic and phonon properties of SrPt₃P under pressure and partial replacement of P by Si, using first-principles method. When pressure increases from 0 to 0.7 Gpa the electron phonon coupling and T_c increases, the calculated T_c agrees with the experiments. For the doped case, SrPt₃P_{0.5}Si_{0.5}, an additional hole pocket around M point in Brillouin zone is formed, almost all the phonon modes shifts into lower energy, and the density of states at the Fermi level decreases, which may explains the drop in T_c observed experimentally.

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