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Structural Stability Driven by the Spin-Orbit Coupling and the Superconductivity in simple-cubic Polonium CHANG-JONG KANG, KYOO KIM, B.I. MIN, POSTECH — Polonium is the only element which has the simple-cubic (SC) structure in the periodic table. We have studied its structural stability based on the phonon dispersion calculations using the first-principles all-electron full-potential band method. We have demonstrated that the strong spin-orbit coupling (SOC) in SC-Po suppresses the Peierls instability and makes the SC structure stable. We have also discussed the structural chirality realized in beta-Po, as a consequence of the phonon instability. Further, we have investigated the possible superconductivity in SC-Po, and predicted that it becomes a superconductor with Tc $\sim$ 4 K at ambient pressure. The transverse soft phonon mode at q $\sim$ 2/3 R, which is greatly affected by the SOC, plays an important role both in the structural stability and the superconductivity in SC-Po. We have explored effects of the SOC and the volume variation on the phonon dispersions and superconducting properties of SC-Po.

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