Pressure-induced electronic and isostructural phase transitions in PdPS: Raman, x-ray, and first-principles study

ABSTRACT

Application of pressure is known to be an effective tool for tuning structural and electronic properties of transition metal dichalcogenides. In this work we present evolution of PdPS with pressure using Raman spectroscopy and synchrotron x-ray diffraction up to 26 GPa, complemented with first-principles theoretical analysis of PdPS under pressure up to 36 GPa. Raman spectra reveal changes in the pressure derivatives of Raman frequencies at P∼2, 11, and 21 GPa, suggesting three isostructural electronic phase transitions in PdPS. The pressure-dependent x-ray diffraction shows a sudden rise in the bulk modulus from 90±3 to 123±7 GPa occurring at P∼11 GPa. Using first-principles density functional theory calculations, we demonstrate that the low-pressure phase transitions are associated with changes in direct band gap at Γ point while the high-pressure (at P=21 GPa) transition is associated with semiconductor to semimetal transition. From analysis of PdPS at higher pressures, we predict a structural phase transition in PdPS at P∼32 GPa from orthorhombic to monoclinic structure.