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Lattice-dynamics of layered HgPSe_3 probed by high-pressure Raman spectroscopy

Pressure-dependent Raman spectroscopy provides a powerful probe of structural instabilities in layered transition-metal phosphorus trichalcogenides, a family of van der Waals materials attracting increasing interest due to their coupled electronic, optical, and lattice properties.^{1,2} In HgPSe_3 , hydrostatic compression induces significant modifications of the vibrational spectrum, revealing the evolution of local bonding and crystal symmetry under pressure.

A clear modification of the Raman spectra occurs between 2.4 and 3.3 GPa, evidenced by mode softening, peak disappearance, intensity redistribution, and mode splitting. These signatures indicate a pressure-induced structural phase transition that precedes the transition detected by X-ray diffraction, highlighting the sensitivity of Raman scattering to local symmetry breaking and bonding distortions. The observed behavior is consistent with pressure-driven structural transitions previously reported in transition-metal phosphorus chalcogenides and related two-dimensional materials.^{3,4}

Lattice-dynamical first-principle calculations based on the density functional theory (DFT) allowed to assign of the observed Raman features and supported the experimentally-observed pressure-induced phase transition from the ambient-pressure monoclinic phase to a centrosymmetric triclinic phase. These findings demonstrate that Raman spectroscopy provides a highly sensitive route for identifying pressure-induced structural evolution in HgPSe_3 and related layered chalcogenides.

References

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Figures

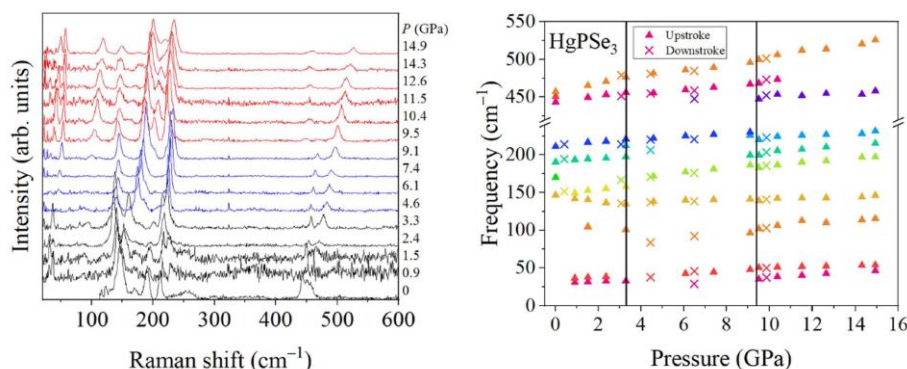


Figure 1: Left: Raman spectra acquired at different pressures, three phases can be identified. Right: Wavenumber of each Raman peak as a function of pressure.