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Pressure induced metallization with absence of structural transition in layered $MoSe_2$ ZHAO ZHAO, Stanford Univ, HAIJUN ZHANG, HONGTAO YUAN, SHIBING WANG, Stanford University, YU LIN, Stanford Univ, QIAOSHI ZENG, ZHENXIAN LIU, Geophysical Laboratory, Carnegie Institution of Washington, KIRIT PATEL, GUNVANT SOLANKI, Sardar Patel University, YI CUI, HAROLD HWANG, WENDY MAO, Stanford University — Layered transition-metal dichalcogenides 2H-MX_2 (M = Mo, W, and etc, X = S, Se, and Te) are emerging as exciting material systems with unique electronic properties and atomically thin geometries. Here, we systematically investigating the high pressure behavior of $2H_c$-$MoSe_2$ up to 60 GPa via a diamond anvil cell, we identified $MoSe_2$ as a promising candidate for lattice and electronic engineering. In sharp contrast to MoS_2, the crystal structure of $MoSe_2$ evolves from an anisotropic two-dimensional layered network to a highly isotropic three-dimensional solid without any structural transition. The role of the chalcogenides anions in stabilizing either $2H_a$ or $2H_c$ layered patterns is underscored by our layer sliding calculations. $MoSe_2$ possesses highly tunable optical and electrical transport properties as a function of pressure, which is essentially determined by the narrowing of its band gap followed by closure at around 40 GPa. Our ab-initio calculations further support the semiconductor to metal transition.

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