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First-principles study of MoHn (n=1, 2 and 3) crystal structures under high pressure XIAOLEI FENG, JURONG ZHANG, Jilin University, HANYU LIU, Carnegie Institution of Washington, HUI WANG, Jilin University — Hydrogen-rich materials have attracted attention recently, owing to their fascinating chemical bonding and potential high superconducting critical temperatures temperature. Inspired by the recent identification of polyhydrides of d metals and molybdenum hydride molecules with a high H content, we explored the crystal structures of MoHn (n = 1, 2, and 3) under high pressures using particle swarm optimization combined with first-principles electronic structure calculations. Several novel structures of MoH2 and MoH3 are predicted at high pressures. MoH is calculated to be stable at ambient pressure; at P $>$ 2.3 GPa the hexagonal phase of MoH2 becomes stable, and at 24 GPa it transforms into an orthorhombic structure, which remains stable up to 100 GPa. All three stable structures show metallic behavior under pressure. The calculated electronic properties suggest that the d-orbitals of the Mo atoms provide the dominant contribution to the density of states at the Fermi level, which is different from the density of states previously predicted for H-rich materials. The present results offer insights in understanding of chemical and physical properties in hydrogen-rich materials, especially in extreme environments.

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