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Pressure-induced phase transitions and superconductivity in platinum hydride[1] CHAO ZHANG, Beijing Computational Science Research Center, XIAOJIA CHEN, Department of Physics, South China University of Technology, HAIQING LIN, Beijing Computational Science Research Center — The transition metal hydrides have attracted much attention from the scientific community due to their promising properties from both fundamental and practical points of view. Here we present our recent work about platinum hydride under pressure. Structural phase transitions and superconducting properties of platinum hydride under pressure are explored through the first-principles calculations based on the density functional theory. Three new low-pressure phases (Pm-3m, Cmmm, and P4/nmm) are predicted, and all of them are metallic and stable relative to decomposed cases. Two high-pressure phases are close-packed structure with hydrogen atoms occupying the octahedral interstices. The superconducting critical temperature of two high-pressure phases correlates with the electron-phonon coupling. The presence of soft modes induced by Kohn anomalies and the hybridization between H and Pt atoms result in the strong electron-phonon coupling. Our results have great implications for other transition metal hydrides under pressure.

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