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First-principles studies of helium in palladium tritides: PdT_x ($0 \leq x \leq 1$) PEI LIN, YAN WANG, M.Y. CHOU, School of Physics, Georgia Institute of Technology — Helium bubbles have significant impact on the stability and mechanical properties of materials used in nuclear-energy systems. Theoretical studies on the behavior of He in various metals have been reported in the past. However, few studies have taken into account the effect of the coexistence of He and tritium (^{3}H) in the metal lattice. We have performed first-principles calculations of He inside palladium tritides with various H concentrations. Instead of interacting with He impurities directly, the interstitial H mainly modifies the electronic structure of the metal lattice. The Pd d-orbital near the Fermi-level shifts downward as H atoms occupy the interstitial sites, which in turn promotes the interaction between He 2-s and Pd 4-d states. We have examined the changes in the formation energy of a He impurity with various H concentrations. The effect will further modify the energetics of trapping multiple He atoms to form a cluster inside the hydrogenated Pd system.

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