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First-principles study of helium bubble formation at a palladium lattice vacancy PEI LIN, YAN WANG, MEI-YIN CHOU, Georgia Institute of Technology — Helium (^{3}He) generated from the tritium decay is one of the main reasons for macroscopic radiation damage in the structural components of nuclear devices such as fission reactors and tritium storage media. In contrast to the hydrogen isotopes, helium with its closed electron shell is inert inside metals and tends to aggregate into bubbles which can cause deterioration of materials and influence the lifetime of reactor components. To examine this behavior, we have performed *ab initio* calculations of helium atoms inside palladium (Pd) using density functional theory (DFT) and the projector augmented wave (PAW) method within the generalized gradient approximation (GGA). We find that He diffuses easily in a defect-free Pd lattice. However, it is energetically favorable for multiple He atoms to be trapped at an isolated Pd vacancy site, forming a cluster of up to 8 atoms. The atomistic mechanisms of He-vacancy interaction in Pd are investigated by studying the corresponding electronic structural properties.

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