

Abstract Submitted
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Monovacancy in hcp-Zirconium Q. PENG, W. JI, Rensselaer Polytechnic Institute, HANCHEN HUANG, University of Connecticut, XIAO-JIA CHEN, Carnegie Institution of Washington, SUVRANU DE, Rensselaer Polytechnic Institute — We investigate the stability of the monovacancy of hcp-Zirconium under various strains by examining the vacancy formation energy through density functional theory calculations. There is a maximum formation energy of monovacancy under uniaxial strain with the value of 0.094 along the c direction, corresponding to a c/a ratio of 1.75. Under volumetric strain, the formation energy decreases with respect to the increment of volumetric strain. The formation energy as a function of pressure was also examined, with a minimum value of 2.00 eV at zero pressure. The formation volume decreases with respect to the pressure, with a value of 0.6 unit-atom-volume at zero pressure particularly. The formation enthalpy increases monotonically as the pressure increases. At a pressure of -15 GPa, the formation enthalpy becomes negative and thus the system fails.

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