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Pressure effect on stabilities of self-Interstitials in HCP-Zirconium QING PENG, WEI JI, JIE LIAN, Rensselaer Polytechnic Institute, XIAO-JIA CHEN, Chinese Academy of Sciences, HANCHEN HUANG, Northeastern University, FEI GAO[1], Pacific Northwest National Laboratory, SUVRANU DE, Rensselaer Polytechnic Institute — The self-interstitial atoms (SIAs) mediate the evolution of micro-structures which is crucial in understanding the instabilities of hexagonal close packed (HCP) structures. Taking zirconium as a prototype, we investigate the pressure effect on the stabilities of SIAs using first-principles calculations based on density-functional theory. We found that the pressure greatly affects the stability of the SIAs. The SIAs in basal planes are more stable under pressure. The SIA configuration of the lowest formation energy changes from basal octahedral (BO) to octahedral (O) at a pressure of 21 GPa. The lowest formation enthalpy configuration switches from BO to S (split-dumbbell) at the pressure of 30 GPa. The formation volumes of SIAs decrease monotonically in response to an increase in pressure. Our results reveal that it is important to take pressure effects into account when predicting the micro-structural evolution of HCP structures. (Scientific Reports, 4, 5735)

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