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Stability and Mobility of Vacancy Defects in Monolayer Graphene[1] WEI CHEN, U of Tennessee-Knoxville, HAIPING LAN, PING CUI, JINLONG YANG, U of Sci. and Tech. of China, ZHENYU ZHANG, Oak Ridge National Lab, U of Tennessee-Knoxville, U of Sci. and Tech. of China — Using DFTB and first-principle calculations, we study the stability and mobility of vacancy defects in graphene. First, we calculate the formation energy of vacancy defects of varying sizes in different supercells, including its dependence on the Brillouin zone sampling. We find a large difference, of 1eV, in the formation energy between the value with only Gamma-point sampling and that with more symmetrical k-point sampling in the 3N*3N (N=2,3,4) supercells. This variance is attributed to significant contributions of the electronic states around the Dirac points. We then explore the mobility of the vacancy defects, including single atom vacancy, trivacancy, and tetravacancy. We find that both trivacancy and tetravacancy have relatively small activation energies for migration via a Stone-Wales transformation of the edge atoms. These results will be compared with recent experimental observations.

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