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Self Healing of Vacancy Defects in Single Layer Graphene and Silicene V. ONGUN OZCELIK, HAKAN GUREL, SALIM CIRACI, Bilkent Univ — Self healing mechanisms of vacancy defects in graphene and silicene are studied using first principles calculations[1]. We investigated host adatom adsorption, diffusion, vacancy formation and revealed atomistic mechanisms in the healing of single, double and triple vacancies of single layer graphene and silicene. Silicon adatom, which is adsorbed to silicene at the top site forms a dumbbell like structure by pushing one Si atom underneath. The asymmetric reconstruction of the single vacancy in graphene is induced by the magnetization through the rebonding of two dangling bonds and acquiring a significant magnetic moment through remaining unsaturated dangling bond. In silicene, three two-fold coordinated atoms surrounding the single vacancy become four-fold coordinated and nonmagnetic through rebonding. The energy gained through new bond formation becomes the driving force for the reconstruction. Under the external supply of host atoms, while the vacancy defects of graphene heal perfectly, Stone-Wales defect can form in the course of healing of silicene vacancy. The electronic and magnetic properties of suspended, single layer graphene and silicene are modified by reconstructed vacancy defects. [1] V. Ongun Ozcelik, H. Gurel, and S. Ciraci, Phys. Rev. B 88, 045440 (2013)].

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