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Diffusion, Coalescence, and Reconstruction of Vacancy Defects in Graphene Layers GUN-DO LEE, EUJJOON YOON, NONG-MOON HWANG, Seoul National University — Recently, vacancy defects in graphene layers have attracted a lot of interest due to the formation of vacancy defects by irradiation, which is the important process in the synthesis of nanotube junctions of various types. In this talk, the diffusion of vacancy defects in single graphene layer is discussed by tight-binding molecular dynamics simulations using the environment-dependent tight-binding carbon potential. We also check the energetics by using ab-initio method. In this study, we find that two single vacancies coalesce into a divacancy and those are reconstructed into a new structure, which is composed of carbon pentagons and heptagons. This reconstructed structure is energetically more favorable than other structures of carbon divacancy. The calculated STM image is compared with experiment. The diffusion of vacancy defects in single-wall carbon nanotubes will also be discussed.

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