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Vacancy Interlayer Migration in Multi-layered Graphene LILI LIU, JUNFENG GAO, Beijing Computational Research Center, XIUYUN ZHANG, Institute of Textiles and Clothing, Hong Kong Polytechnic University, TIANYING YAN, Institute of New Energy Material Chemistry, Nakan University, FENG DING, Institute of Textiles and Clothing, Hong Kong Polytechnic University — Graphene has innumerous applications due to its exceptional properties. Various defects that may be introduced into the graphene lattice during synthesis and/or post-treatments are known have significantly impact on these properties. So engineering graphene by introducing or annealing of defects is an important technology to achieve desired properties for various applications. Therefore a comprehensive understanding on the behavior of defects in graphene is critically important. Here, interlayer migration of the vacancies in multi-layered graphene (MLG) was investigated by density functional tight-binding molecular dynamic simulations and first principle calculations. Our study reveals that, although the direct vacancy migration between neighboring graphene layers (NGLs) is prohibited by a very high barrier up to $\sim$ 7 eV, the interaction between vacancies or vacancy and holes in NGLs can greatly reduce the barrier to $\sim$ 3 eV and expedites the migration process. Our study reveals a new mechanism of the defect self-healing in MLG and multi-walled carbon nanotubes and it can be used to engineer desired graphene materials.

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