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Self-healing and adsorbate-induced removal of defects on graphene and carbon nanotubes LEONIDAS TSETSERIS, Vanderbilt University and University of Thessaloniki (Greece), SOKRATES PANTELIDES, Vanderbilt University and Oak Ridge National Laboratory — The presence of point defects is known to induce significant changes in the electronic, chemical, transport, and mechanical properties of graphitic systems. Here, we use first-principles calculations based on density-functional theory to describe several adatom-related processes that alter key physical traits of graphene and carbon nanotubes. We find that, while pairs of C adatoms and clusters of four or more self-interstitials stay idle unless the system is heated to very high temperatures, clustering of three C adatoms leads to removal of hillock-like features and creates mobile species, resulting in self-healing of defective structures. We also demonstrate the reactivity of defect pairs using hydrogen and oxygen as prototype adsorbates, and we show that interaction with extrinsic species is an alternative healing mechanism for adatom structures in the above systems. The results relate to the evolution of defects either during growth of carbon nanotubes or during post-growth treatment and operation of related devices. This work was supported in part by DOE Grant DEFG0203ER46096.

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