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Chemical reactions and thermal stability of oxygen impurities on graphene[1] BIN WANG, Department of Physics and Astronomy, Vanderbilt University, SOKRATES PANTELIDES, Vanderbilt University and ORNL — Oxygen as an impurity is known to degrade conductivity in graphene, but annealing at moderate temperature reverses the effect. Here we report first-principles calculations of oxygen binding and reactions on graphene that elucidate the underlying physics. We find that two O atoms can form an O dimer that can desorb from graphene with an overall activation barrier of 1.3 eV. Oxygen can also be removed in a more complicated reaction in which C atoms in graphene are consumed. We find that structural defects such as Stone-Wales defect and grain boundaries show enhanced binding to O atoms due to the local strain, facilitating the O reaction. If H atoms coexist, an O atom can bind to an H atom forming an OH group, which can also be removed by thermal annealing due to the weak binding, resulting in defect-free graphene.

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