Graphene in the presence of impurities and defects
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Graphene, a single layer of carbon structure graphite, has a number of interesting electronic properties. To aid in the understanding of these properties, we have performed first-principles calculations of graphene in the presence of impurities such as Fe and Br. We analyze the lattice distortions, electronic structures and spin states of these systems. In addition, calculations and analysis involving defects such as single and double vacancies and Stone-Wales defects are also performed.