Exploring point defects in hexagonal boron-nitrogen monolayers

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A comprehensive theoretical study of selected point defects for monolayers of hexagonal boron nitride (h-BN) is presented. Two-dimensional structures were simulated through h-BN flakes built from thirty-six up more than one hundred boron and nitrogen atoms and used to examine various defects, like: atom vacancies, atom substitutions, or distortions of the hexagonal lattice. Since carbon contaminations are very common in the h-BN technology, a particular attention has been paid to carbon impurities. The calculations of IR spectra in the harmonic approximation for the doped flakes reveals the presence of additional frequencies, which in many cases correspond to defect-bound modes. In particular, when two carbon atoms are close to each other, a localized stretching C-C mode of a high intensity has been found, with a frequency value of about 100-200 cm^{-1} higher than for collective B-N stretch frequencies. UV-Vis spectra obtained from time-dependent density functional theory show that the inclusion of impurities results in an emergence of several low-energy electronic excitations, from which some are localized on a defect, while other are delocalized. Energies of these excitations are strongly dependent on the defect type, and they range from about 0.7 to 6.1 eV for the lowest excitations, while for the undoped h-BN flake the lowest transition of about 6.1 eV with zero intensity has been found, in agreement with recent experimental and theoretical values for the h-BN band gap. Based on the calculated UV-Vis and IR spectra we propose several defects, which could be responsible for the experimental 4 eV color band. These candidates are the defects built from two or four adjacent carbon atoms, for which the lowest electronic excitation of the excitation energy ranging from 3.9 to 4.8 eV is localized on a defect.

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