Structure and energetics of the vacancy in graphite

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We determine the structure and energetics of the point defects in graphite from first principles calculations. The Jahn–Teller effect takes place at low temperature, breaking the symmetry and lowering the vacancy formation energy. This results in a weak in–plane reconstruction bond between two of the unsaturated atoms surrounding the vacancy and the displacement of the remaining unsaturated atom out of the plane. This last feature of the distortion increases the interaction of the vacancy with other defects, affecting its migration energy. We comment on the STM images of the symmetric and asymmetric vacancy and also the significance of these findings in understanding defect behaviour in irradiated graphite and related graphitic materials, in particular single walled nanotubes.