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Vacancy Complexes in Carbon and Boron Nitride Nanotubes

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ABSTRACT

The effect of divacancies on the stability, structural and electronic properties of carbon and boron nitride nanotubes is studied using the *ab initio* density functional method. V_BB_N is more stable in the boron-rich and less stable in the nitrogen-rich growth conditions, and V_NN_B is more stable in the nitrogen-rich than in the boron-rich conditions. We find that stoichiometric defects V_BV_N,V_BC_N and V_NC_B are stable in both the boron and nitrogen rich environments. The relaxation energy in the V_CV_C is lower in the armchair than in the zig-zag and the opposite trend is seen for V_CB_C and V_CN_C. The divacancy is found to be particularly effective in changing the band gap of the semiconducting nanotubes due to the appearance of additional energy levels within the band gap region. For the zig-zag systems, we observe a drastic reduction of the band gap in V_BB_N,V_NN_B and V_NC_B and a complete removal of the band gap in V_BV_N and V_BC_N, negating the semiconducting behaviour of the nanotube.