ABSTRACT

The effect of divacancies on the stability, structural and electronic properties of carbon and boron nitride nanotubes is studied using the \textit{ab initio} density functional method. $V_B B_N$ is more stable in the boron-rich and less stable in the nitrogen-rich growth conditions, and $V_N N_B$ is more stable in the nitrogen-rich than in the boron-rich conditions. We find that stoichiometric defects $V_B V_N$, $V_B C_N$ and $V_N C_B$ are stable in both the boron and nitrogen rich environments. The relaxation energy in the $V_B V_C$ is lower in the armchair than in the zig-zag and the opposite trend is seen for $V_N B_C$ and $V_C N_C$. 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 $V_B B_N$, $V_N N_B$ and $V_N C_B$ and a complete removal of the band gap in $V_B V_N$ and $V_B C_N$, negating the semiconducting behaviour of the nanotube.