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Ab initio studies of isolated boron substitutional defects in graphane

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Abstract content
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We have systematically studied the energetics, electronic and structural properties of various configurations of B substituting CH pair located on a single hexagonal ring of graphane using first-principles calculations. The number of substitutional defects considered ranges from one to six B dopants and isomers are formed by choosing different doping sites for the same number of dopants. Based on the formation energy analysis, we found that isomers differ significantly in relative stability. For instance, meta and para isomers (B defects surrounded by C atoms) are energetically favourable, whereas the formation of B - B bond (ortho) is unstable. The density of states show a transition from semiconductor to metallic with increasing number of B dopants. This modulation of band gap, to a great extent, is an indication that B-doped graphane systems can be exploited for band gap-related applications.

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