The effect of Electron doping in non magnetic YH_3 Leading to Room Temperature Ferromagnetism and Flat Band: Insights from Density functional theory

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Supplementary information:-

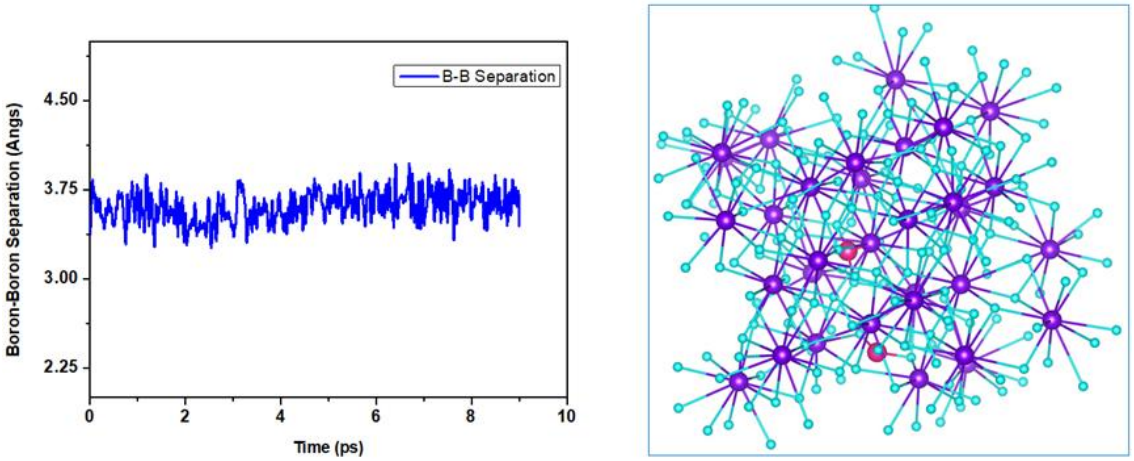

Figure-S1 **Fluctuations in B-B separation Structural snap shot at 300 K, and 3.57Å separation, after 10 ps with 2 Boron atoms substitution as obtained from AIMD simulations**

With the increasing B-B separation, the total energy may not change monotonically as there may be different magnetic interactions at different separation, e.g, superexchange interactions, Zener double exchangeinteractions, RKKY interaction etc. Different mechanisms valid at different regime. If we see ΔE, the energy difference between AFM and FM state it is maximum of 0.27 eV (of the order of 0.1 eV as mentioned by the reviewer), which is the magnetic interaction energy but the total energy difference between different B-B configuration is around 7-8 eV, which comes due to interactions between electrons and ions. The large energy difference between different B-B configurations implies that if we start with particular B-B separations, it is unlikely to get another B-B separation.

This justifies that chances of B-B clustering is less as energy of starting B-B configuration differs from other B-B configuration. We have done AIMD simulations at 300 K and found that fluctuations in B-B separation are very less even after 10 ps.

So there is less chance of B-B clustering as B atoms are substituted in place of H atom and bonded in the environment by Y atom and other H atoms.Different B-B separation corresponds to different impurity concentration. The idea of studying different B-B separation is to find the configuration for which the energy difference between AFM and FM state is maximum. Experimentalist can choose the impurity concentration corresponding to that B-B separation to maximize ΔE as well as Curie temperature. But once a particular B-B separation choose, B-B atoms are unlikely to get clustered due higher energy barriers as well as the fact that B atoms are not ad atoms, but bonded on the site with Y and other H atoms.

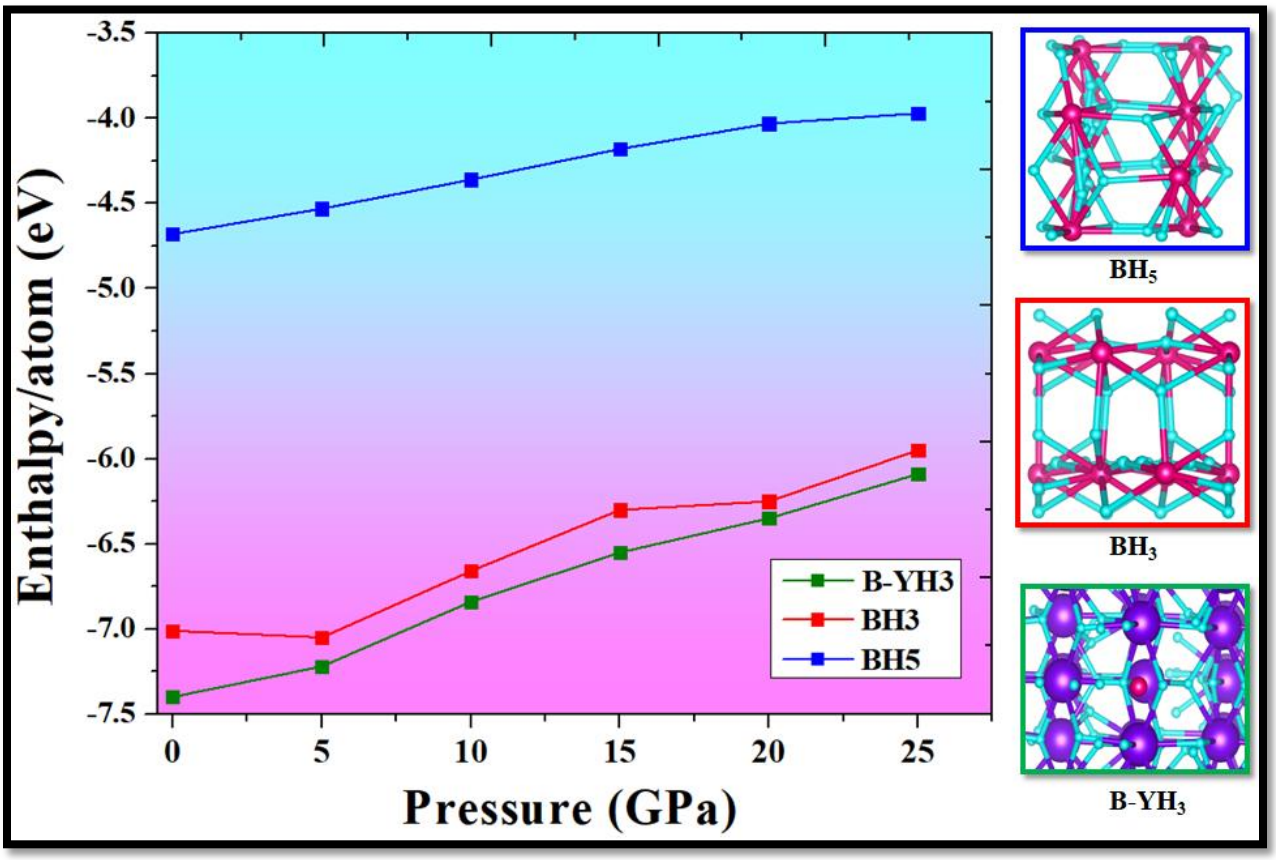

Figure S-2: DFT calculated enthalpy as a function of pressure for the DFT-GGA calculations between the pressure range 0–25GPa for BH_3, BH_5, and B-YH_3