Exploring the Size-Dependent Hydrogen Storage Property on Ti-Doped B_n Clusters by Diatomic Deposition: Temperature Controlled H_2 Release

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Abstract
The hydrogen storage properties of Ti-doped B_n ((Formula presented.)) clusters are investigated by using the “diatomic deposition method” with further evaluation by density functional theory computations. The results show that TiB_n ((Formula presented.)) clusters possess the ability to storage up to four H_2 molecules, reaching a mass fraction of 6.12%. Further, the hydrogen release temperature is analyzed by molecular dynamics simulations with a variable temperature. It turns out that the TiB_7 and TiB_9 clusters release the H_2 molecules at $T \lesssim 700$ K, while TiB_8 requires higher temperature due to stronger interactions with the H_2 molecules, confirmed by the electronic density of states. The size-dependent properties and odd–even nuclearity on the clusters can be useful for applications with controlled temperature. These results serve for further design of novel materials with reversible and controlled hydrogen storage properties based on TiB_7/TiB_9 motifs. Additionally, new lower-energy isomers for TiB_4 and TiB_9 clusters were found within the accuracy of the all-electron triple-ζ Slater [slater type orbital (STO)-Triple-zeta basis set(TZP)] basis set.

Author keywords
boron clusters
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