Hydrogen Storage Capacity of Be2(NLi)2 Cluster with Ultra-short Beryllium-Beryllium Distance

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Abstract

Quantum chemical calculations have been carried out to investigate the hydrogen storage capacity of Be2(NLi)2 cluster which contains ultra-short beryllium-beryllium distance. Calculations reveal that the cluster can take up to 6 H2 molecules reaching a maximum gravimetric density of 16.6 wt%. All the H2 binds at the Li atom with a moderate binding energy which is required for reversible storage of H2. Symmetry adapted perturbation analysis reveals significant contribution of electrostatic and induction and very minor contribution of dispersion towards the total interaction energy. The interaction between the H2 and Li centre is found to possess significant covalency. Molecular dynamics simulations reveal that the H2 molecules are strongly bound at 77K and get slowly released at elevated temperature.

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