Revisiting the world of metal nitrides for hydrogen storage applications – A DFT study

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Abstract

Efficient storage of hydrogen is one serious impediment in using H2as an alternate clean fuel, at a larger scale, in the context of alarming levels of global warming and fast depleting fossil fuel resources.Metal nitrides such as Li2N4, Na2N4 and K2N4using density functional theory at PBE1PBE and B3LYP functional using 6-31G (d,p), 6-31++G (d,p) and 6-311++G (d,p) as basis sets have revealed that doping of alkali-metal atoms on the nitride systems increases their hydrogen adsorption ability, due to electron transfer that occurs from the metal atom to the nitrogen surface. The charged surface created around the metal atom is found to enhance the hydrogen adsorption capacity of the complex from 9 to 16.79wt% with an average binding energy of0.06 to 0.30 eV/H2. Various conceptual reactivity descriptors,bond parameters, Gibbs free energy change (ΔG) and energy gap values, support the ideathat the stability of the complex increaseson hydrogen uptake.

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