

DFT STUDY OF THE STRUCTURE, STABILITY AND ELEMENTARY REACTIONS OF SIMPLE AND COMPLEX HYDRIDES OF LIGHT ELEMENTS

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Review of results of DFT calculations of potential energy surfaces, structures, energetic and spectroscopic properties, and elementary reactions of sorption-desorption of molecular hydrogen in tetrahydroborates and alanates of light elements, in doped aluminum clusters, fullerenes, and other complexes with high content of active hydrogen, which have been carried out in our Lab for the last few years. The B3LYP/6-31G* approach and (for the simplest and modeling systems) the more sophisticated coupled cluster method CCSD(T)/6-311+G** have been used as “working” computational approximations. Following topics will be discussed in detail:

1. The structure and energetic stability of borate and alanate molecules $M(\text{BH}_4)_n$ and $M(\text{AlH}_4)_n$ of the light *sp*-elements and 3*d*-transitional metals. Energies and potential barriers of H_2 molecule cleavage and their tendencies in related series.

2. The potential energy surfaces of elementary chemisorption reactions of H_2 and light (CH_4 , C_2H_6) alkane molecules on doped aluminum clusters LAl_{12} with dopants $\text{L} = \text{B}, \text{C}, \text{Si}, \text{Ge}, \text{Ti}$, and some other light 3*d*-metals located inside and at the periphery of the Al_{12} cage. Dependence of energies and potential barriers of these reactions on the nature and position of dopant, on external charge and multiplicity of electronic states. Minimal energy pathways and energies of step-wise (successive) hydrogenation of aluminum clusters.

3. The structure and stability of hypothetical neutral and charged complexes $M(\text{H}_2)_n$ with high ($n = 6 - 8$ and more) numbers of H_2 molecules inside the coordination sphere of 3*d*-metal atoms and ions.

4. Hydrogenated fullerenes. Modelling of the structure, properties and elementary reactions of

simple hydrides (CH_4 , BH_4^- , AlH_4^- , C_2H_2 , etc) confined under high-pressure conditions inside the tight and “superlight” pristine and hydrogenated fullerene cages of various size and form.

References

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