Poster Presentation

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BH4 cluster ordering in complex metal borohydrides

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Complex borohydride compounds attract an increasing interest as hydrogen storage materials. Although they have been investigated for more than fifty years, there is still a lot of unknown physical phenomena awaiting to be revealed regarding, for example the dynamics and ordering of BH4 clusters in different borohydrides. The orientation of BH4 unit with respect to the surrounding metallic atoms is unique for a particular metal and determines e.g. the crystal space group, total energy of a system and the potential freedom of BH4 movement, like rotations, within the crystal structure. The information about rotations is of great importance for understanding how the hydrogen atoms behave in such systems [1,2]. To gain a closer look on how the borohydride clusters can rotate, their geometrical arrangement has been studied using analysis of tensor of inertia (TI). Free BH4 takes the form of a regular tetrahedron, but when it is placed among metal atoms, a compound is formed, in which certain deformation of this tetrahedral atomic arrangement may take place. Here the TI analysis turns out to be an efficient tool, since it might reveal how the BH4 deformation influences its rotational freedom, by analyzing the principal moments of inertia and principal eigenvectors corresponding to them, which are in fact, the most probable rotation axes. In the paper a comprehensive study is presented and the possible axes of rotation in complex metal borohydrides MBH4 (M=Li, Na, Ca, K, Mn, Rb, Cs, Sr, Zr), are discussed. For a given metal borohydride TI is performed on both experimentally obtained structures and predicted by theoretical calculations. A comparison of these results gives an insight into how the theory reflects real measurements and what discrepancies or similarities are observed.

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