AB-INITIO STUDY OF THE GROUP 2 HYDRIDE ANIONS

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The beryllium hydride $(Be\cdots H)^-$ dimer has recently[a] been shown to be surprisingly strongly bound, with an electronic structure which is highly dependent on internuclear separation. At the equilibrium distance, the negative charge is to be found on the beryllium atom, despite the higher electronegativity of the hydrogen. The current study expands this investigation to the other Group 2 hydrides, and attempts to explain these effects.

[a] M. Verdicchio, G. L. Bendazzoli, S. Evangelisti, T. Leininger *J. Phys. Chem. A*, **117**, 192, (2013)