Bonding in Zintl phase hydrides: Density functional calculations for $SrAlSiH$, $SrAl_2H_2$, $SrGa_2H_2$ and $BaGa_2H_2$

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We investigate the bonding characteristics of SrAlSiH, $SrAl_2H_2$, $SrGa_2H_2$ and $BaGa_2H_2$ using density functional calculations. Zintl type mixed bonding is found, with the formation of covalent sp^2 bonds in the Al/Ga/Al-Si planes of the various compounds. On the other hand the Sr and Ba atoms occur as divalent cations, while the H is effectively anionic.