

# Theoretical design of stable hydride clusters: isoelectronic transformation in the $E_nAl_4H_{7+n}$ series

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New stable hydrogen-rich metallic hydrides are designed by systematic transformations of the stable known  $Al_4H_7^-$  species, carried out by successive isoelectronic substitutions of one aluminum atom by one E-H unit at a time (where E = Be, Mg, Ca, Sr and Ba atoms). Searches on the potential energy surfaces (PESs) of  $EAl_3H_8^-$ ,  $E_2Al_2H_9^-$ ,  $E_3AlH_{10}^-$  and  $E_4H_{11}^-$  systems indicate that structural analogues of  $Al_4H_7^-$  become higher energy isomers as the number of E-H units increases. The electronic descriptors: Vertical Electron Affinity (VEA), Vertical Ionization Potential (VIP) and the HOMO-LUMO gap, suggest that the systems composed of  $EAl_3H_8^-$ ,  $E_2Al_2H_9^-$ ,  $E_3AlH_{10}^-$ , with E = Be and Mg, would be the most stable clusters. Additionally, for a practical application, we found that the Be-H and Mg-H substitutions increase the hydrogen weight percentage (wt%) in the clusters, compared with the isoelectronic analogue  $Al_4H_7^-$ . The good capacity of beryllium and magnesium to stabilize the extra hydrogen atoms is supported by the increment of the bridge-like E-H-Al, 3center-2electron chemical bonds. Finally, explorations on the PESs of the neutral species (using  $Na^+$  as counterion) indicate that the  $NaBe_2Al_2H_9$ ,  $NaBe_3AlH_{10}$  and  $NaMg_3AlH_{10}$  minimum-energy structures retain the original geometric shapes of the anionic systems. This analysis supports the potential use of these species as building blocks for cluster-assembled hydrides in the gas phase. © The Royal Society of Chemistry.