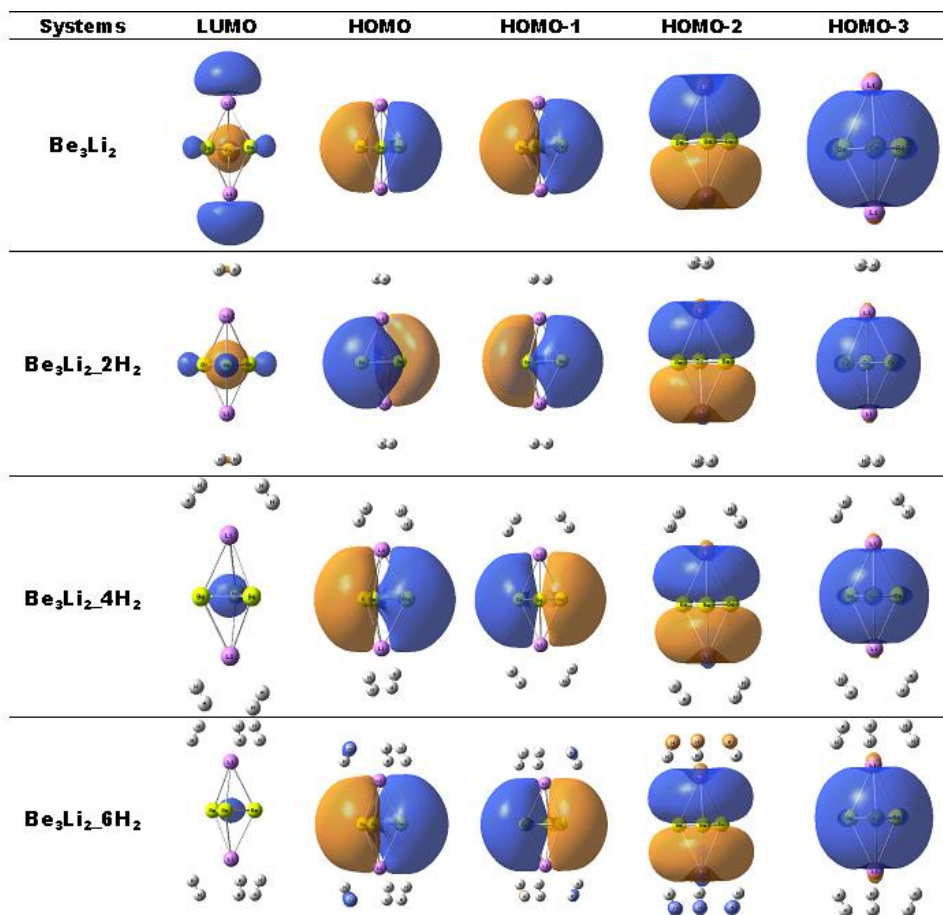
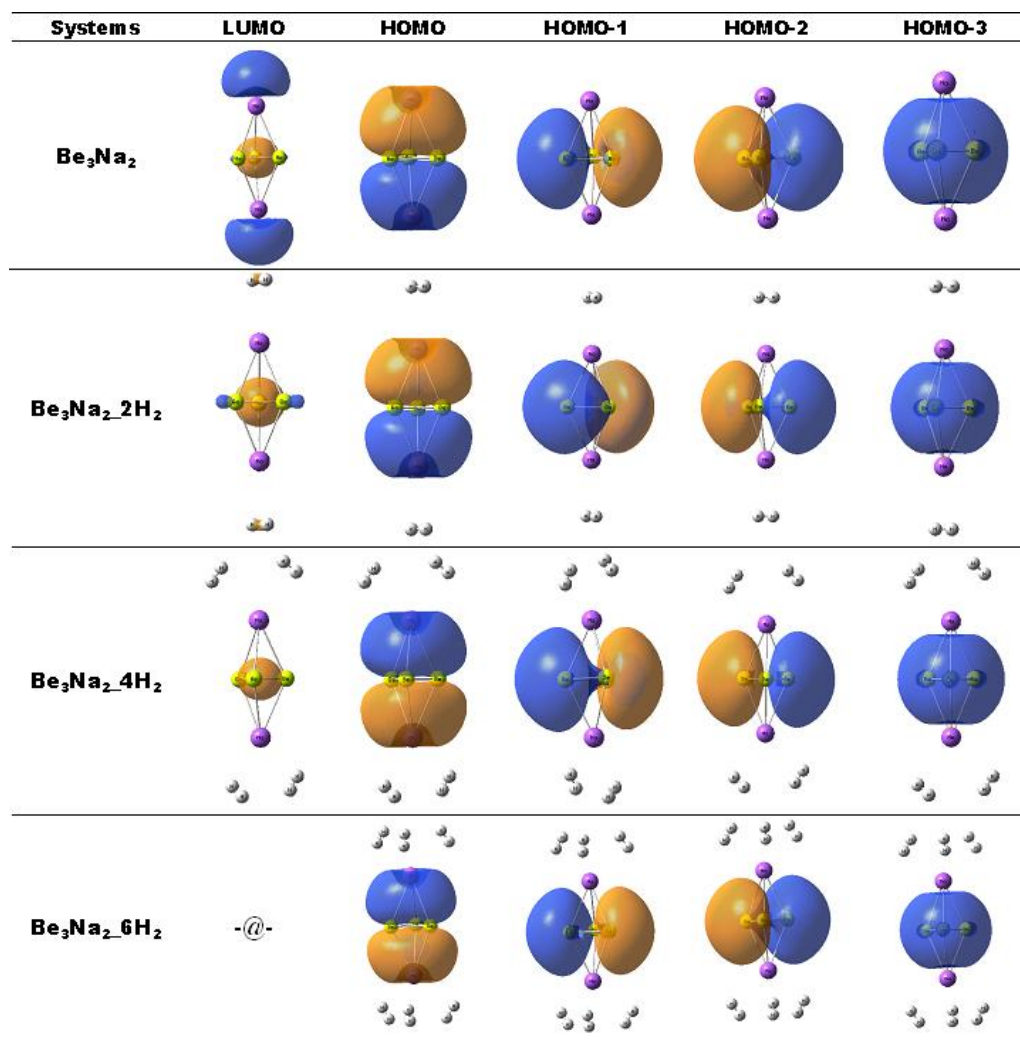


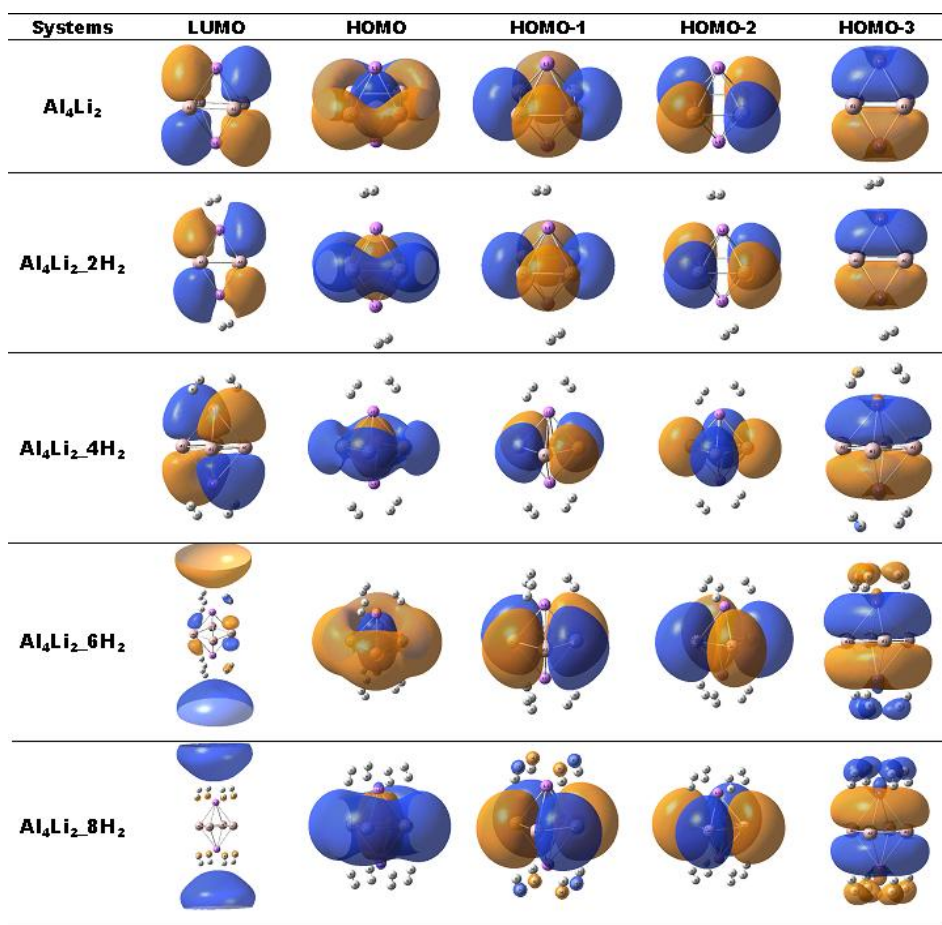
**Figure S1.** Variation of NICS (0) and NICS (1) for H<sub>2</sub> trapped Al<sub>4</sub>Li<sub>2</sub> systems in triplet state with increase in the number of adsorbed molecular hydrogen.



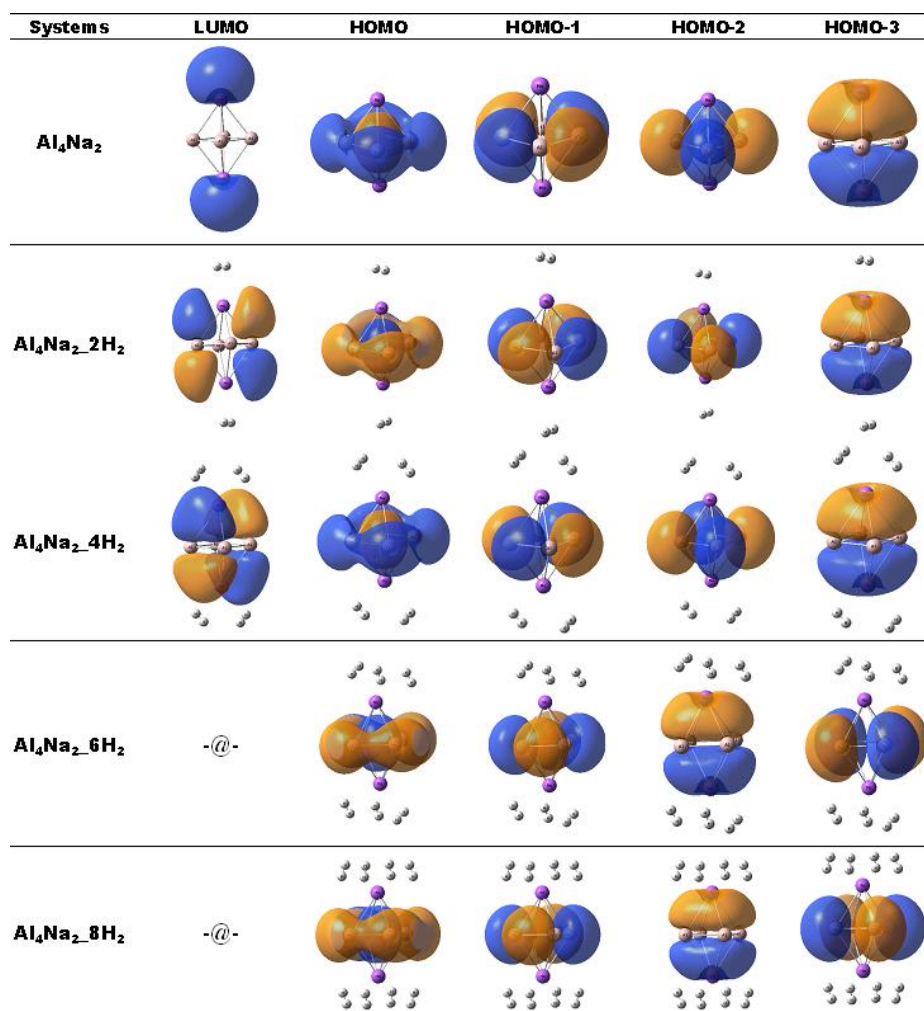
**Fig. S2.** Frontier molecular orbital (FMO) pictures of  $\text{Be}_3\text{Li}_2$  and  $\text{Be}_3\text{Li}_2(\text{H}_2)_{2n}$  generated at iso-value 0.02



**Fig. S3.** Frontier molecular orbital (FMO) pictures of Be<sub>3</sub>Na<sub>2</sub> and Be<sub>3</sub>Na<sub>2</sub>(H<sub>2</sub>)<sub>2n</sub> generated at isovalue 0.02.  
 -@- not generated in GaussView



**Fig. S4.** Frontier molecular orbital (FMO) pictures of  $\text{Al}_4\text{Li}_2$  and  $\text{Al}_4\text{Li}_2(\text{H}_2)_{2n}$  generated at isovalue 0.02



**Fig. S5.** Frontier molecular orbital (FMO) pictures of  $\text{Al}_4\text{Na}_2$  and  $\text{Al}_4\text{Na}_2(\text{H}_2)_{2n}$  generated at isovalue 0.02.

-@- not generated in GaussView