

## Electronic Supplementary Information

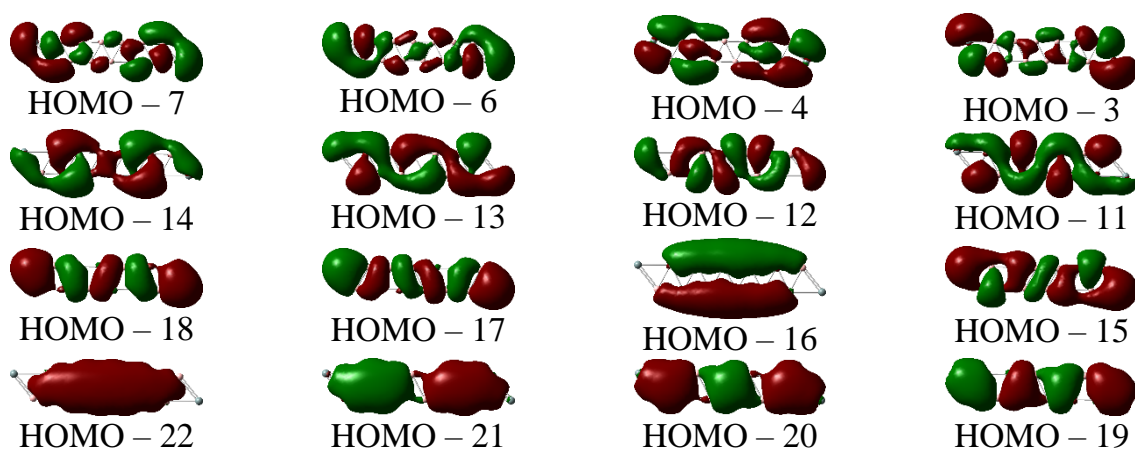
### Silicon doped boron clusters: how to make stable ribbons?

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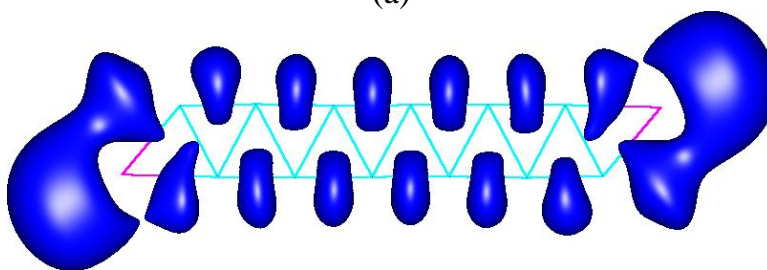
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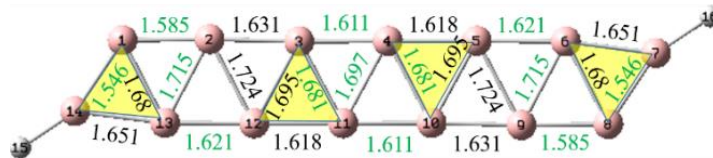


(a)

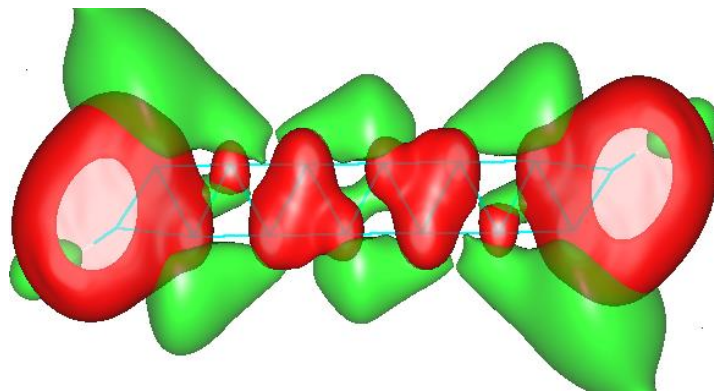


(b)

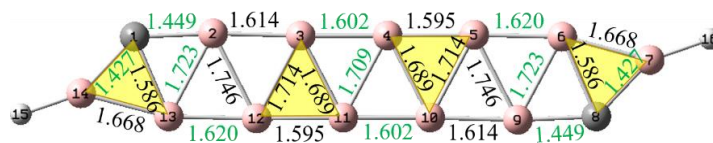
**Figure S1.** a) 16 localized CMOs and b) the ELF( $\sigma_{\text{loc}}$ ) of  $\text{B}_{12}\text{Si}_2^{2-}$ .



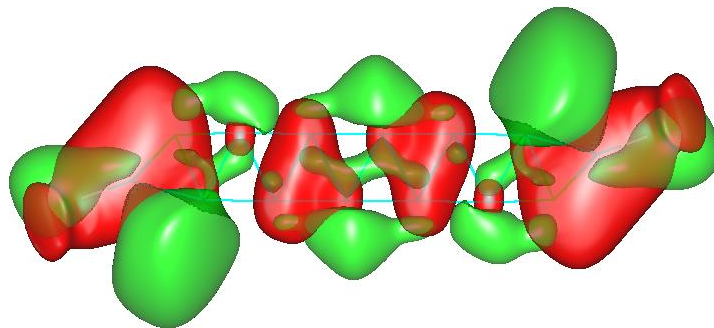
a)  $B_{14}H_2^{2-}$



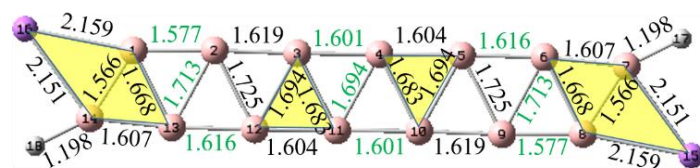
b) ELF( $\pi$ ) and ELF( $\sigma_{delo}$ ) for the  $B_{14}H_2^{2-}$



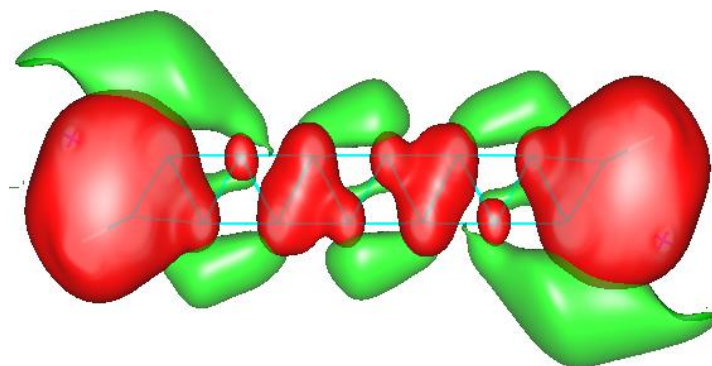
c)  $B_{12}C_2H_2$



d) ELF( $\pi$ ) and ELF( $\sigma_{delo}$ ) for the  $B_{12}C_2H_2$

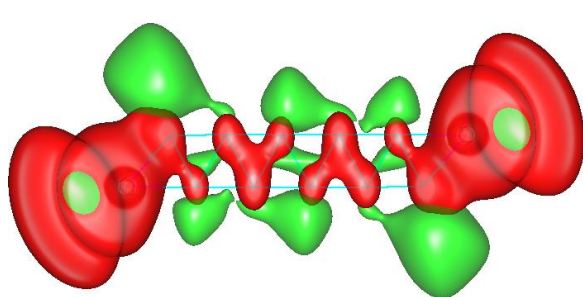


e)  $B_{14}Li_2H_2$

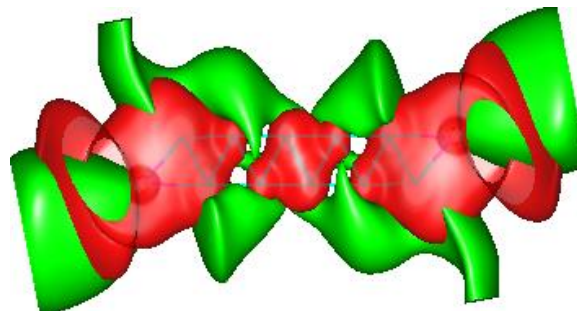


f) ELF( $\pi$ ) and ELF( $\sigma_{delo}$ ) for the  $B_{14}Li_2H_2$

**Figure S2.** Ribbon structures of (a)  $B_{14}H_2^{2-}$ , (c)  $B_{12}C_2H_2$ , and (e)  $B_{14}Li_2H_2$ . The ELF( $\pi$ ) (red) and ELF( $\sigma_{delo}$ ) (green) are plotted simultaneously for (b) the  $B_{14}H_2^{2-}$ , (d)  $B_{12}C_2H_2$  and (f)  $B_{14}Li_2H_2$ . The bond length ( $\text{\AA}$ ) is given in Figures (a), (c), and (e). Yellow areas indicate places affected by  $\pi$  delocalized electrons while green bonds are affected by  $\sigma$  delocalized electrons.

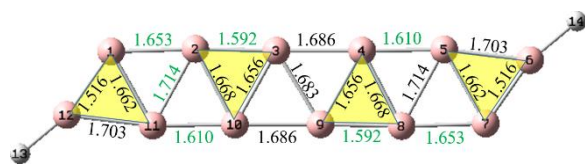


a) ELF( $\pi$ ) and ELF( $\sigma_{delo}$ ) for the  $\alpha$  spin electrons of  $B_{10}Si_2^{2-}$  triplet

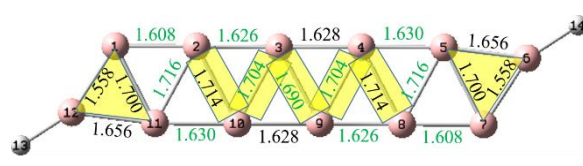


b) ELF( $\pi$ ) and ELF( $\sigma_{delo}$ ) for the  $\beta$  spin electrons of  $B_{10}Si_2^{2-}$  triplet

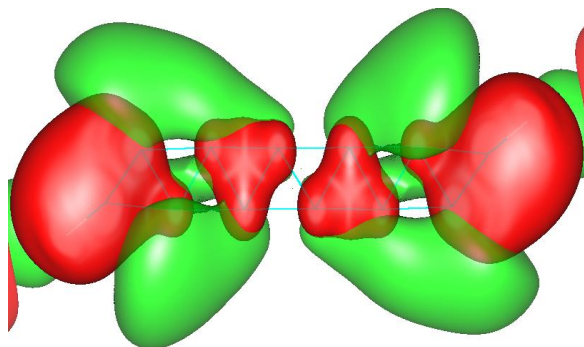
**Figure S3.** The ELF( $\pi$ ) (red) and ELF( $\sigma_{delo}$ ) (green) are plotted simultaneously for (a)  $\alpha$  spin electrons, and (b)  $\beta$  spin electrons of triplet  $B_{10}Si_2^{2-}$ .



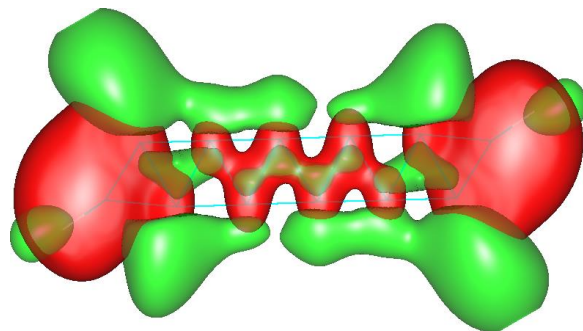
a)  $B_{12}H_2^{2-}$  singlet



c)  $B_{12}H_2^{2-}$  triplet

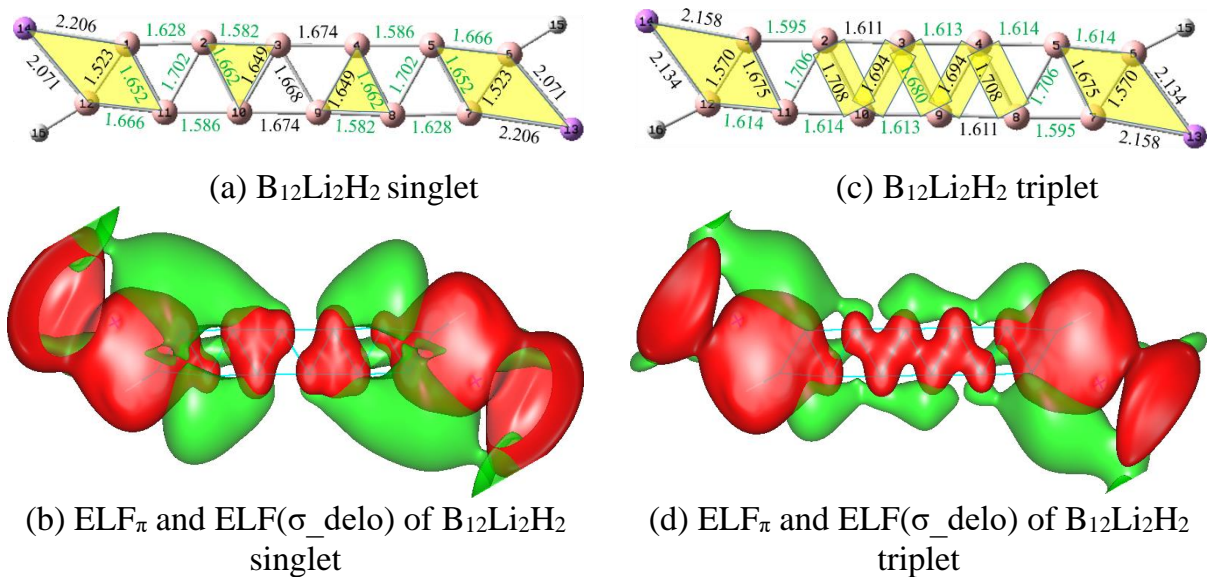


b) ELF( $\pi$ ) and ELF( $\sigma_{delo}$ ) of  $B_{12}H_2^{2-}$  singlet

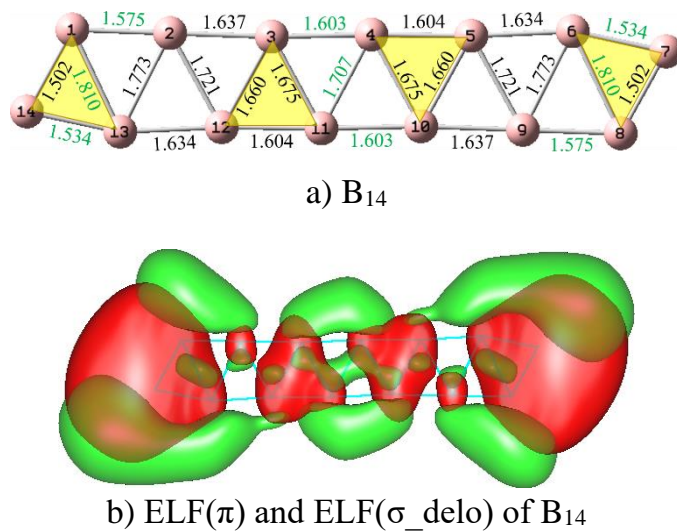


d) ELF( $\pi$ ) and ELF( $\sigma_{delo}$ ) of  $B_{12}H_2^{2-}$  triplet

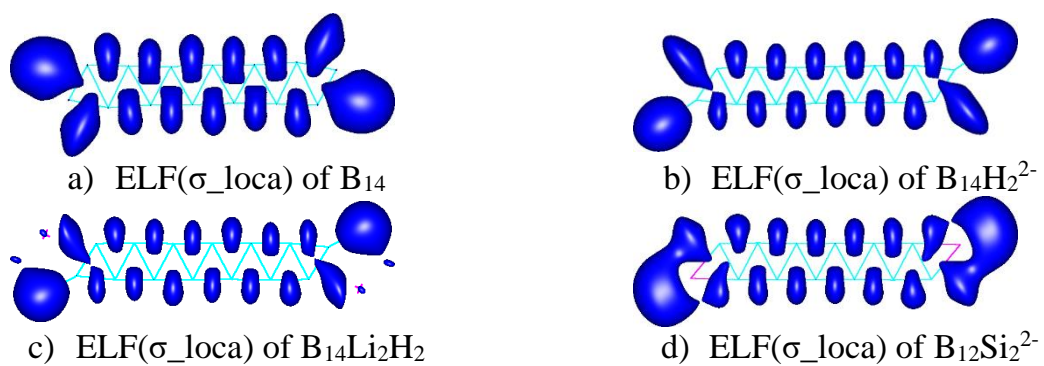
**Figure S4.** Ribbon structure of  $B_{12}H_2^{2-}$  in (a) singlet and (c) triplet states. ELF( $\pi$ ) (red) and ELF( $\sigma_{delo}$ ) (green) are plotted simultaneously for (b) singlet  $B_{10}H_2^{2-}$  and (d) triplet  $B_{10}H_2^{2-}$ . Bond lengths ( $\text{\AA}$ ) are given in Figure (a) and (c). Yellow areas indicate the places affected by  $\pi$  delocalized electrons while green bonds are effected by  $\sigma$  delocalized electrons.



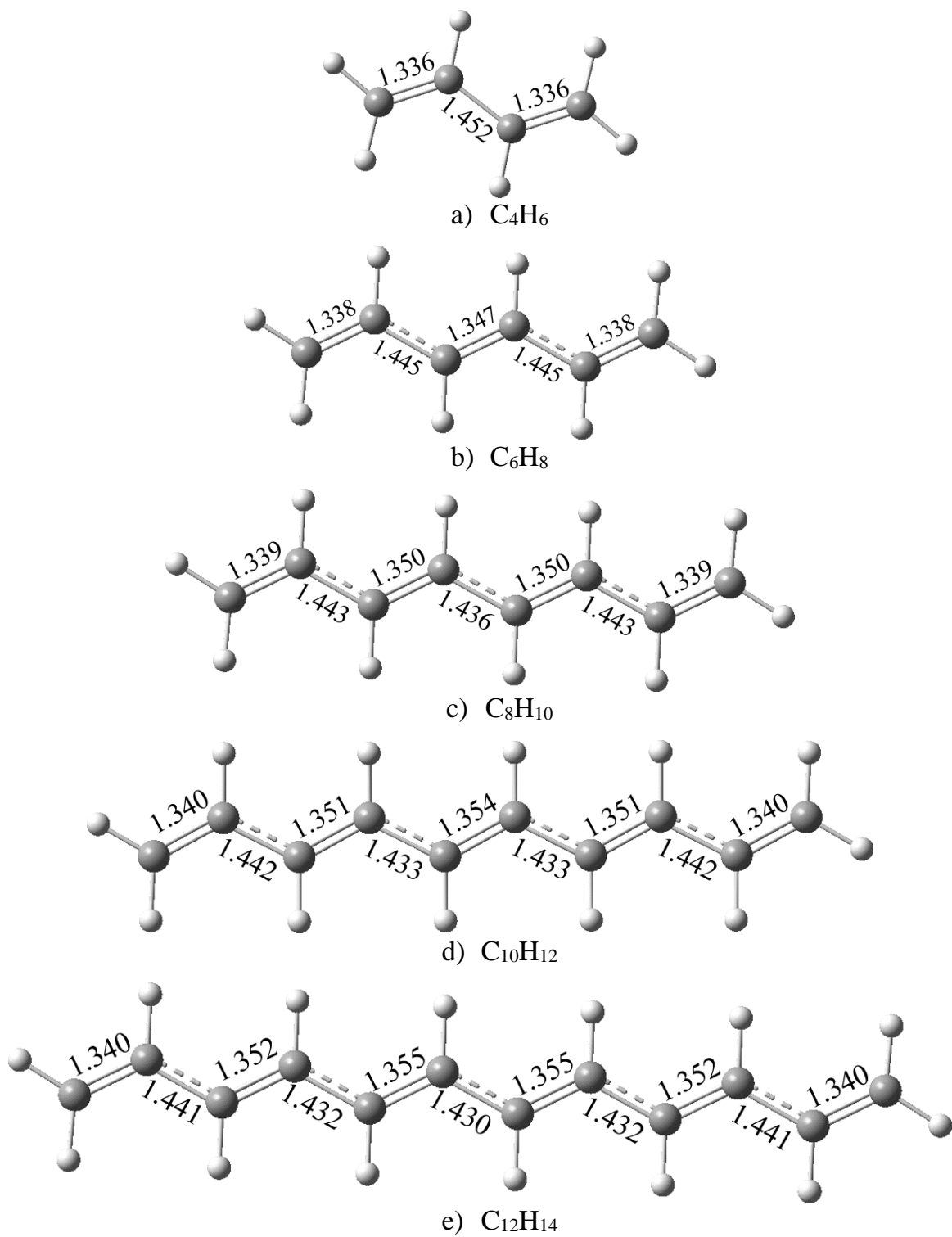
**Figure S5.** Ribbon structure of  $B_{12}Li_2H_2$  in (a) singlet and (c) triplet states.  $ELF(\pi)$  (red) and  $ELF(\sigma_{delo})$  (green) are plotted simultaneously for (b) singlet  $B_{12}Li_2H_2$  and (d) triplet  $B_{12}Li_2H_2$ . Bond lengths (Å) are given in Figure (a) and (c). Yellow areas indicate the places affected by  $\pi$  delocalized electrons while green bonds are effected by  $\sigma$  delocalized electrons.



**Figure S6.** Ribbon structure of  $B_{14}$ .  $ELF(\pi)$  (red) and  $ELF(\sigma_{delo})$  (green) are plotted simultaneously for (b) singlet  $B_{12}Li_2H_2$  and (d) triplet  $B_{12}Li_2H_2$ . Bond lengths (Å) are given in Figure (a) and (c). Yellow areas indicate the places affected by  $\pi$  delocalized electrons while green bonds are effected by  $\sigma$  delocalized electrons.



**Figure S7.** The ELF( $\sigma_{loca}$ ) of (a)  $B_{14}$ , (b)  $B_{14}H_2^{2-}$ , (c)  $B_{14}Li_2H_2^{2-}$ , and (d)  $B_{12}Si_2^{2-}$ .



**Figure S8.** Optimized structures of (a)  $C_4H_6$ , (b)  $C_6H_8$ , (c)  $C_8H_{10}$ , (d)  $C_{10}H_{12}$ , and (e)  $C_{12}H_{14}$  using DFT with the PBE1 functional and the 6-311+G(d,p) basis set.