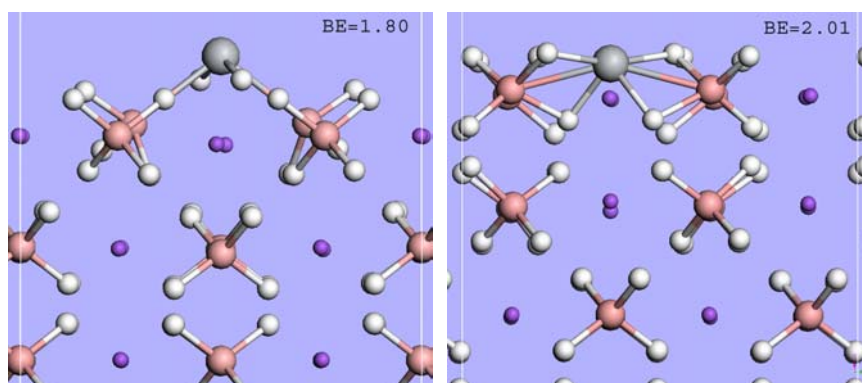
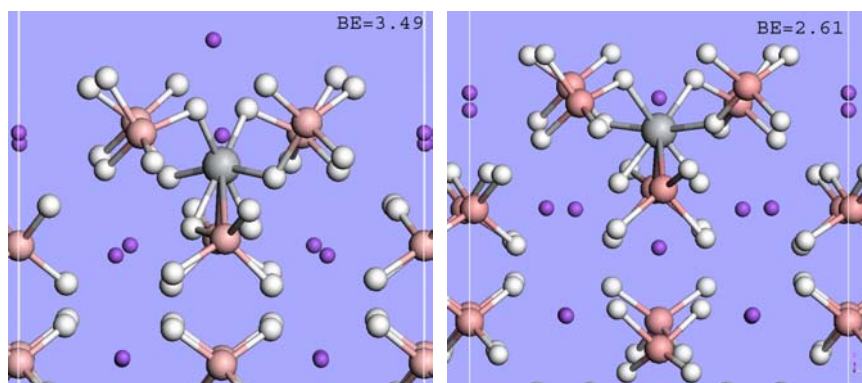


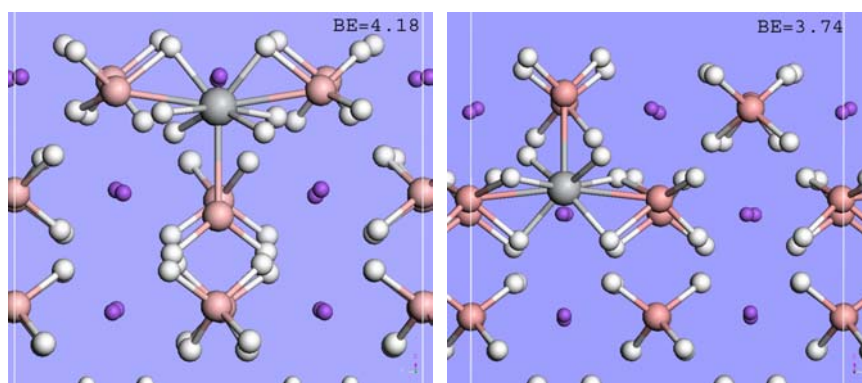
Supplementary information: GGA-relaxed structures and binding energies of Ti in Ti-doped NaAlH₄(001) with Ti occupying various possible positions. (a) Ti adsorbed on the surface and connected with two neighboring AlH₄⁻ hydrides. (b) Ti substitutes lattice Na⁺ and pushes Na upward or downward. (c) Ti occupies interstitial site and binds three neighboring AlH₄⁻ hydrides. Binding energies (in eV) are labeled in the corresponding structure.



(a)



(b)



(c)