

Restructuring and Hydrogen Evolution on Sub-nanosized Pd_xB_y Clusters

Supplementary Materials

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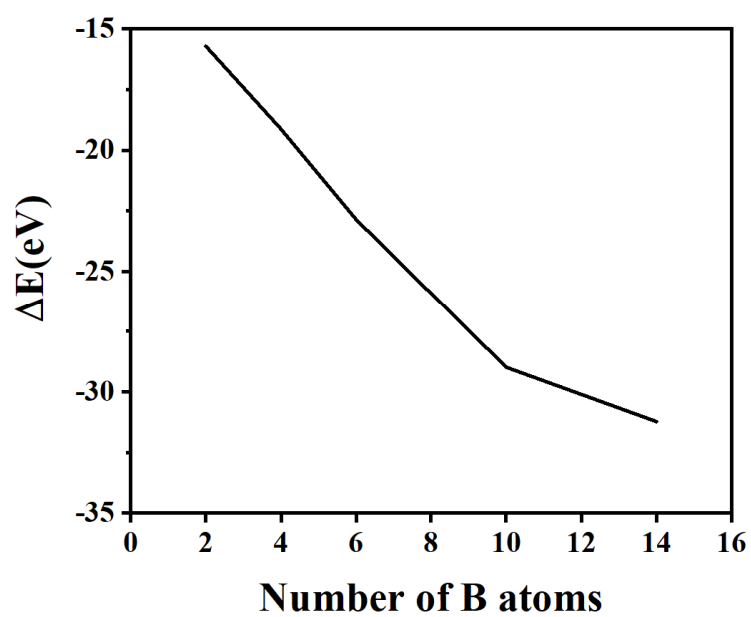


Figure S1. The decrease of GM energy (ΔE) of the most stable cluster varies with the number of B atoms.

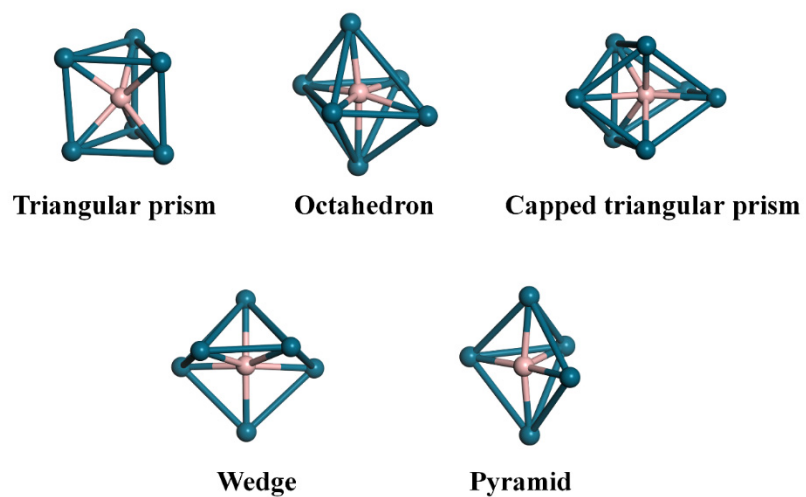


Figure S2. Coordination geometry of B atoms in Pd_xB_y GM clusters (deep-blue ball presents Pd atom, pink ball presents B atom).

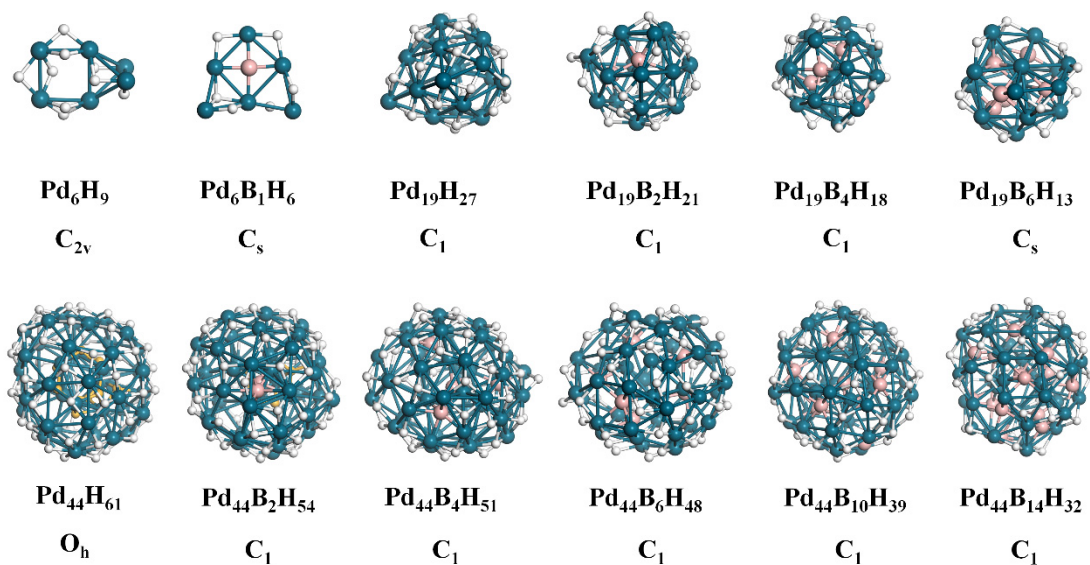


Figure S3. GM structures of Pd_xB_yH_z clusters under HER conditions with their symmetry of Pd sub-structure (deep-blue ball presents Pd atom, pink ball presents B atom, white ball presents H atom on cluster surface, and orange ball presents H atom siting inner of the cluster).

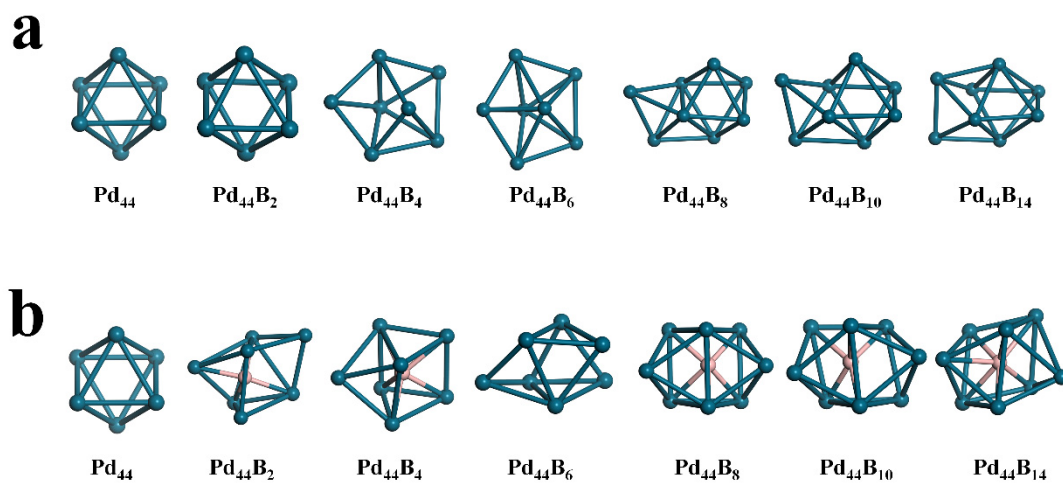


Figure S4. Changes of core structures in Pd_{44}B_y clusters. (a) The core structures in Pd_xB_y clusters. (b) The core structures in $\text{Pd}_x\text{B}_y\text{H}_z$ clusters under HER conditions.

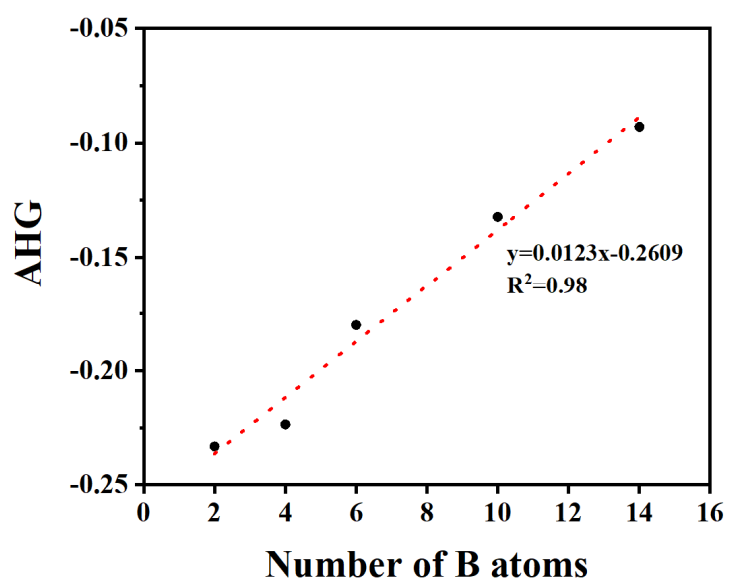


Figure S5. The change of average H adsorption free energy (AHG) of Pd₄₄B_yH_z GM structures with the number of B atoms, and red line is its linear fitting.

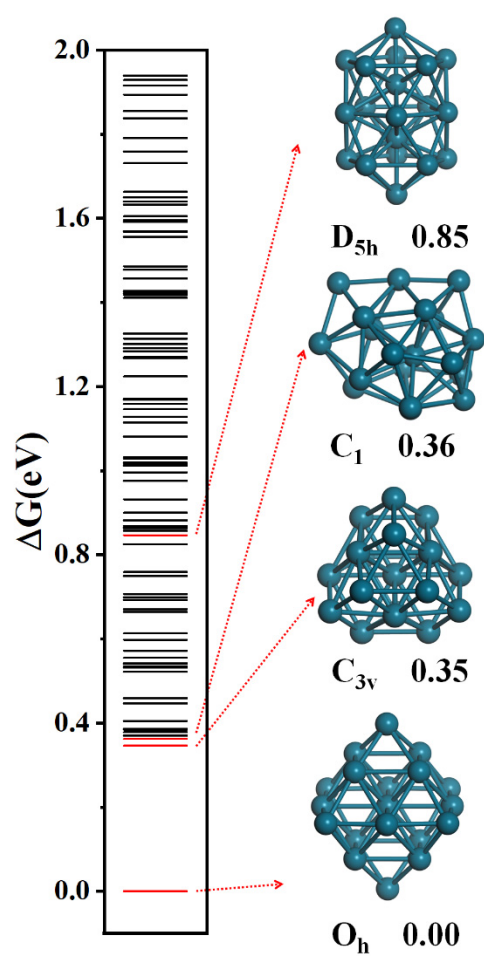


Figure S6. Low-lying isomers diagram of Pd₁₉ clusters.

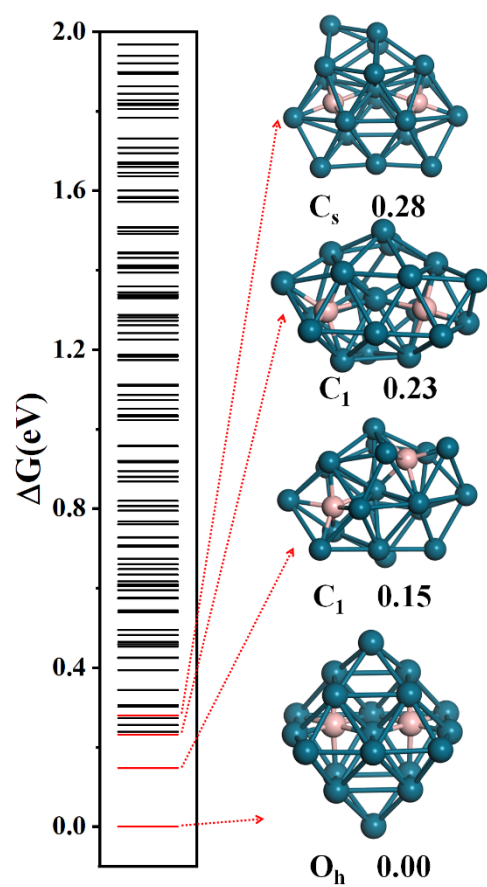


Figure S7. Low-lying isomers diagram of Pd_{19}B_2 clusters.

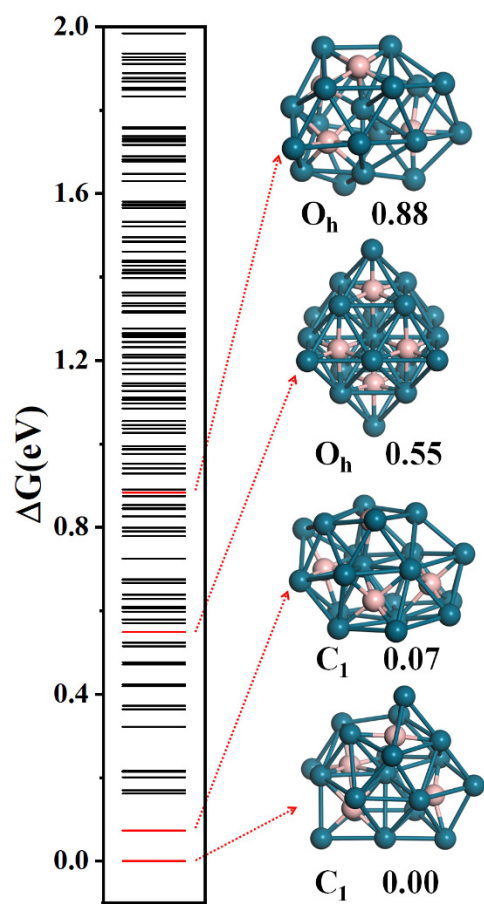


Figure S8. Low-lying isomers diagram of Pd_{19}B_4 clusters.

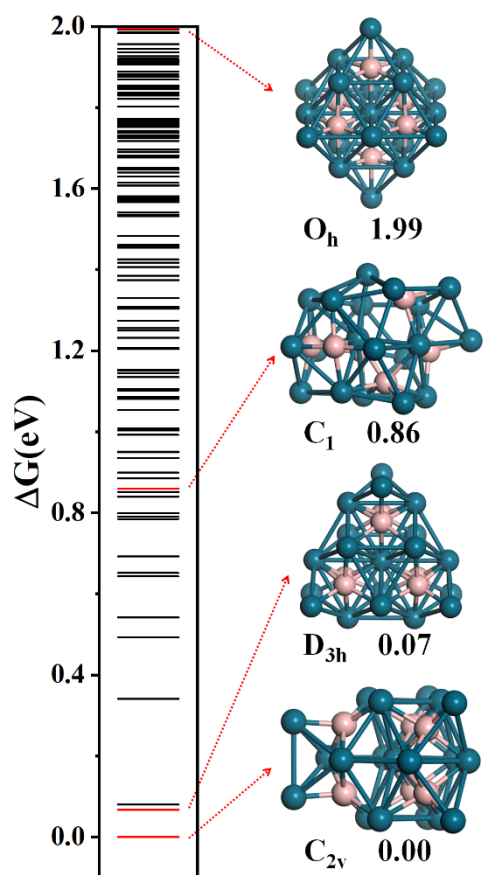


Figure S9. Low-lying isomers diagram of Pd_{19}B_6 clusters.

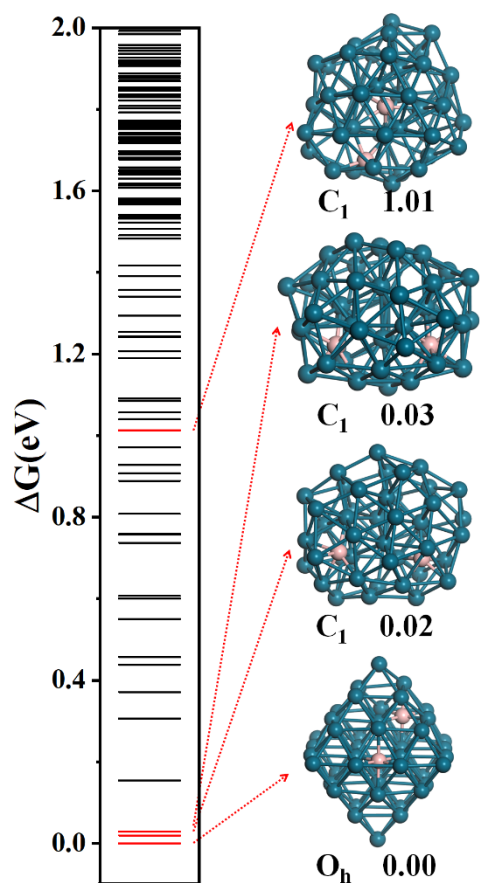


Figure S10. Low-lying isomers diagram of Pd_{44}B_2 clusters.

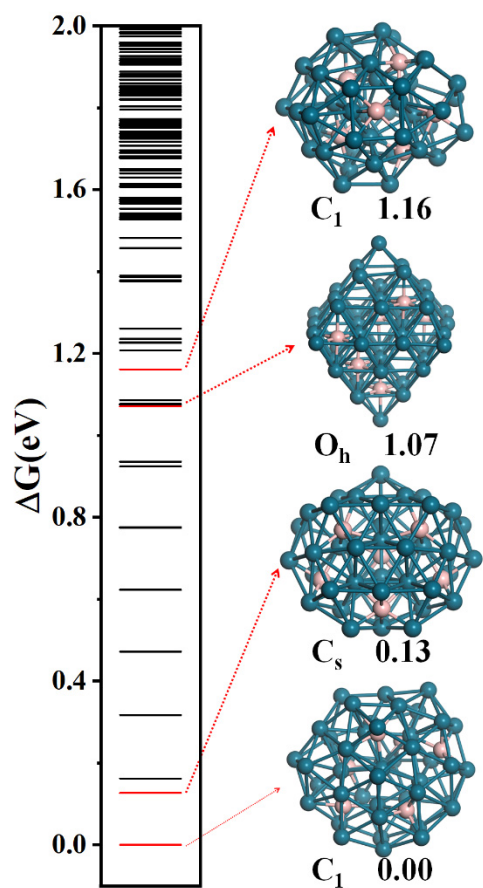


Figure S11. Low-lying isomers diagram of Pd_{44}B_6 clusters.

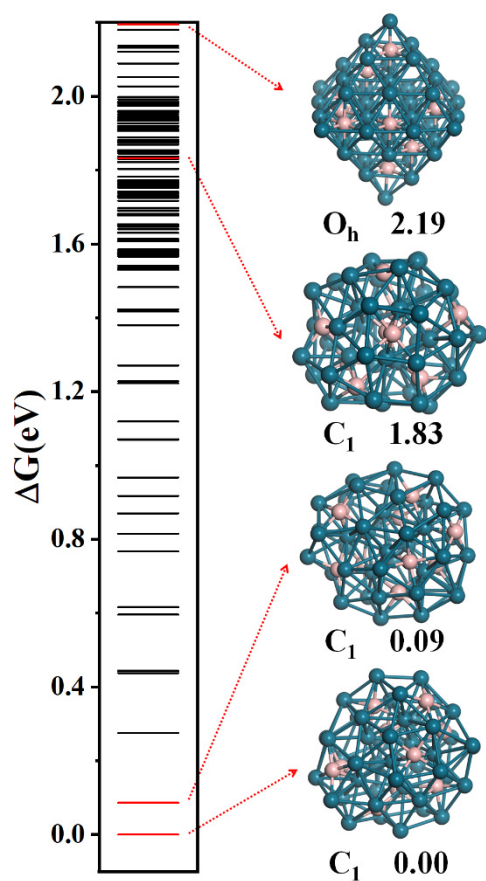


Figure S12. Low-lying isomers diagram of $\text{Pd}_{44}\text{B}_{10}$ clusters.

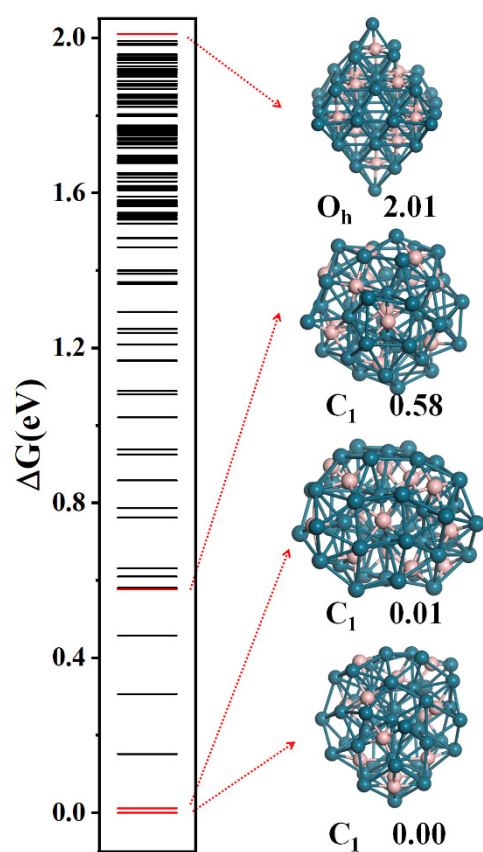


Figure S13. Low-lying isomers diagram of $\text{Pd}_{44}\text{B}_{14}$ clusters.

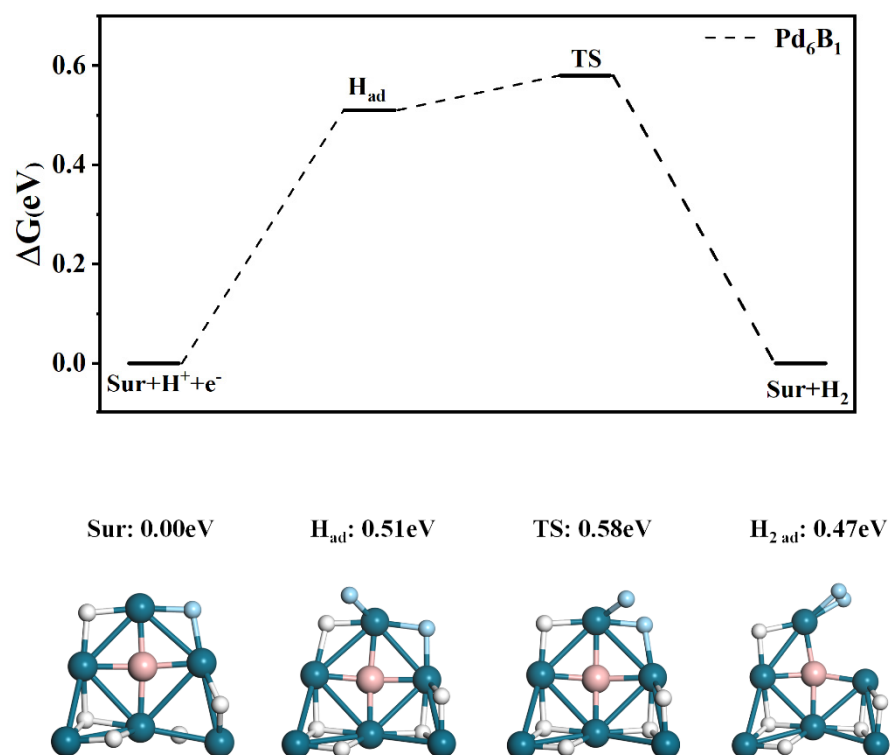


Figure S14. The HER energy diagram of Pd_6B cluster, and structures of every step during HER pathway.

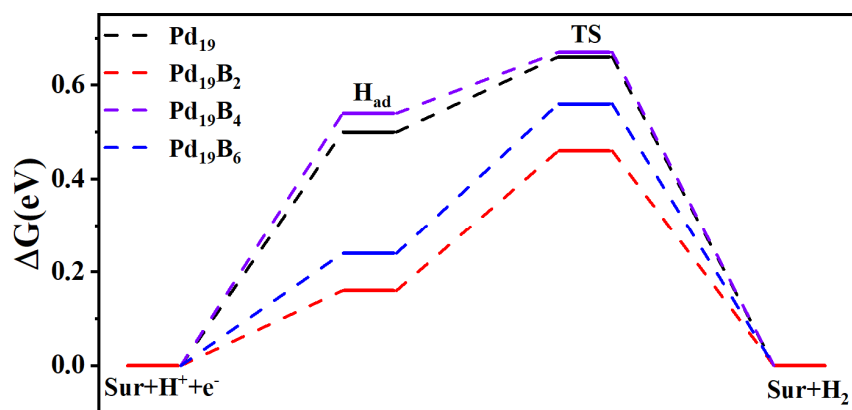


Figure S15. The HER energy diagram of Pd_{19}B_y ($y=0,2,4,6$) clusters.

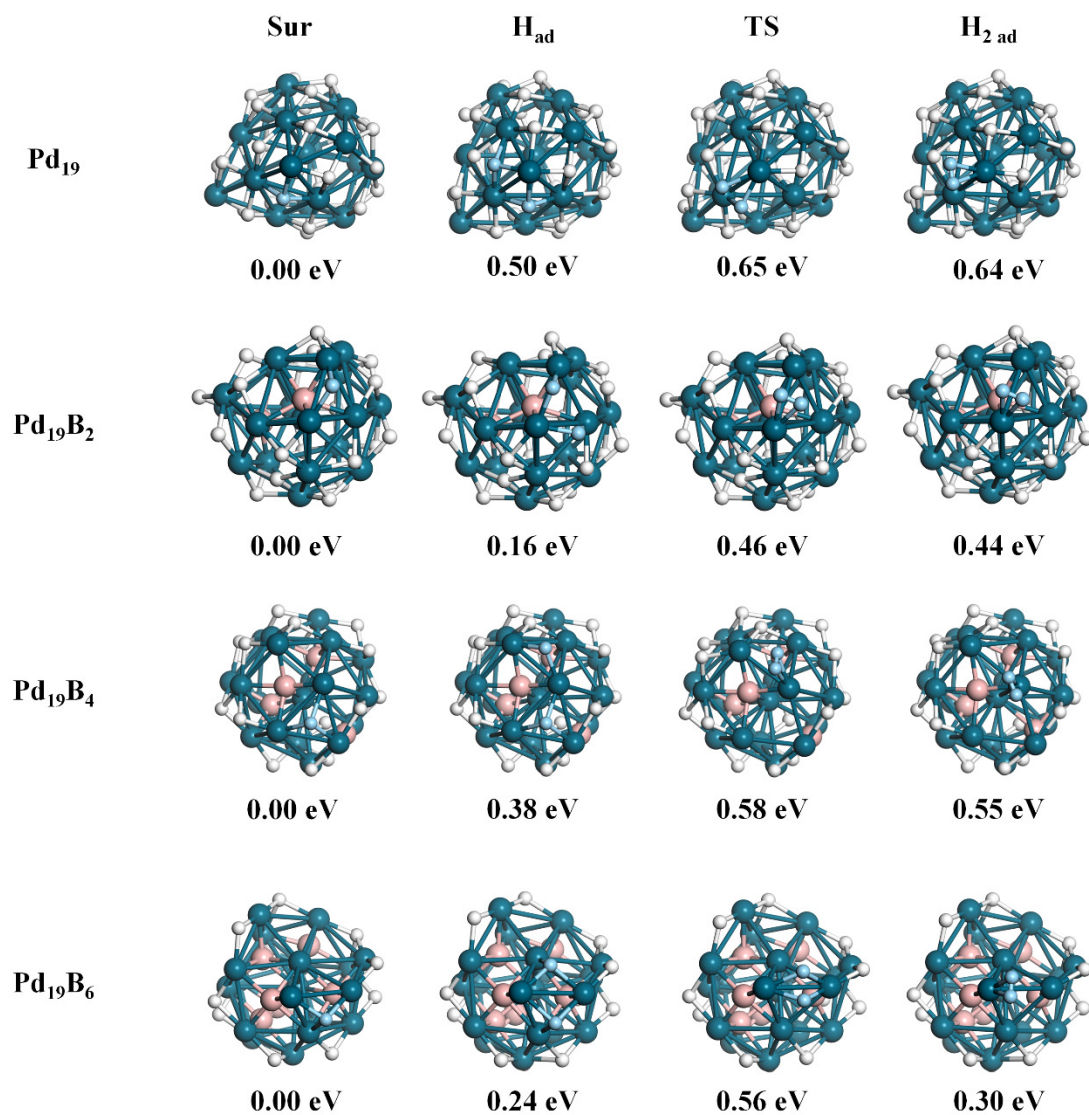


Figure S16. The structures of every step during HER pathway for Pd₁₉B_y (y=0,2,4,6) clusters.

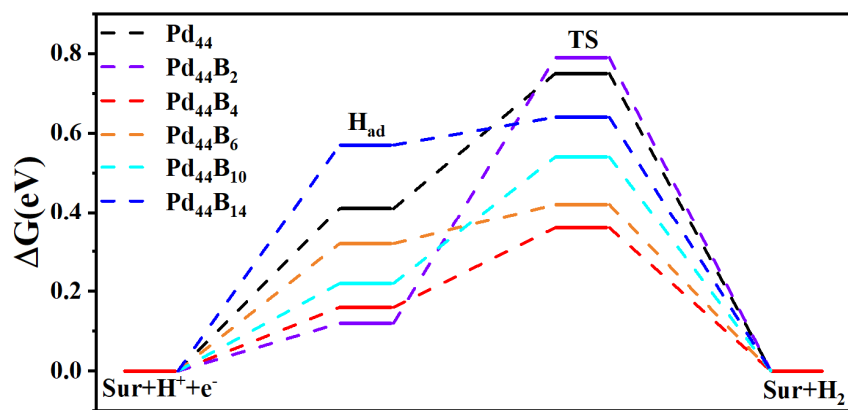


Figure S17. The HER energy diagram of Pd₄₄B_y (y=0,2,4,6,10,14) clusters.

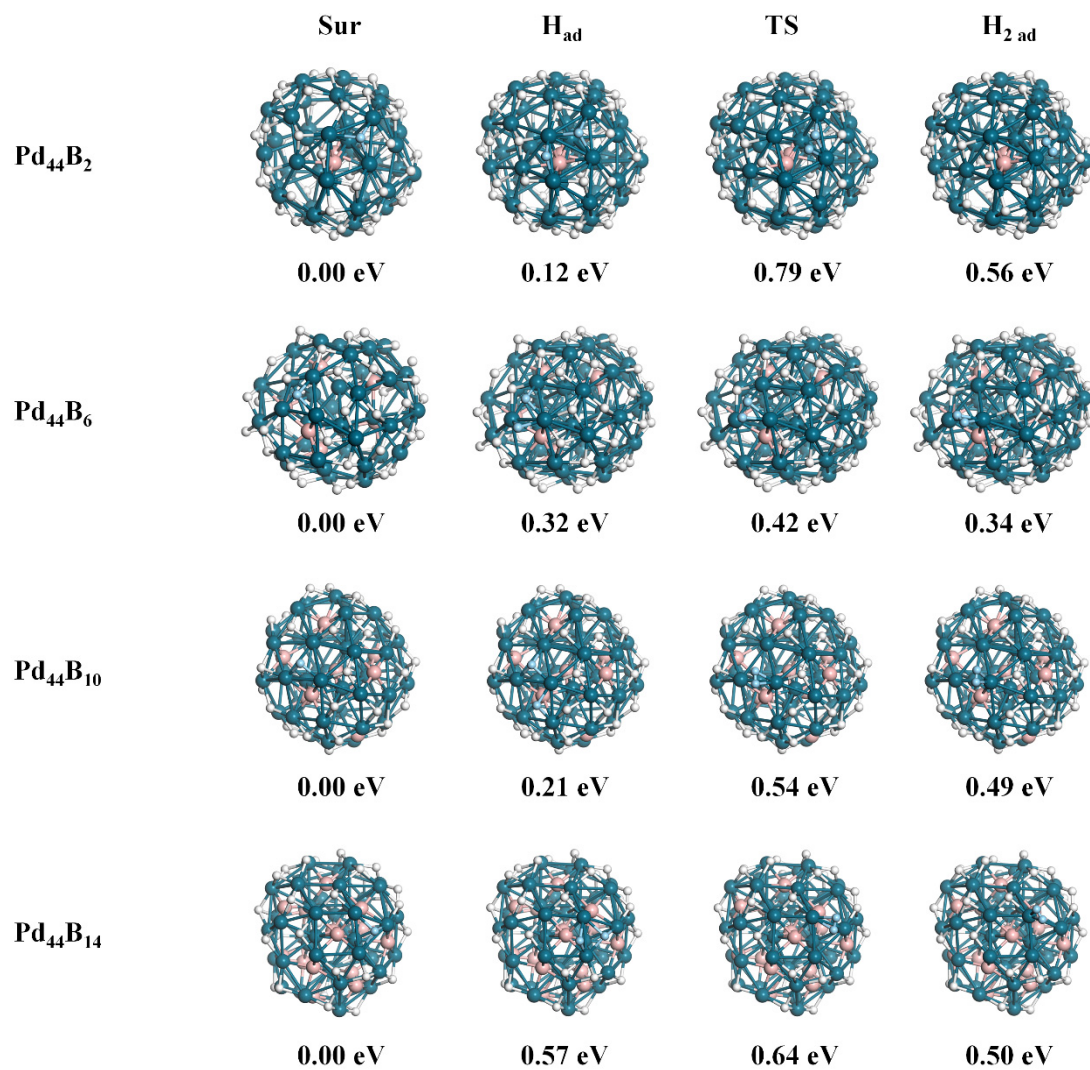


Figure S18. The structures of every step during HER pathway for Pd₁₉B_y (y=2,6,10,14) clusters.

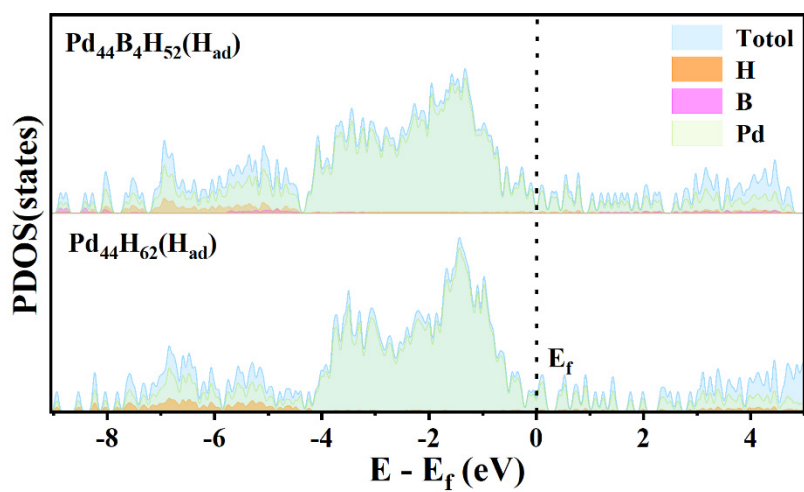


Figure S19. Partial wave density of state (PDOS) of $\text{Pd}_{44}\text{B}_4\text{H}_{52}$ and $\text{Pd}_{44}\text{H}_{62}$ (H_{ad} state for HER).