

To understand how water molecules are adsorbed by clusters. After we scan the potential energy surface between the adsorbed water molecule clusters, the specific results are shown in Figure S1, Figure S2, Figure S3, Figure S4, Figure S5. The results show that the adsorption reaction has no energy barrier.

Flexible scanning

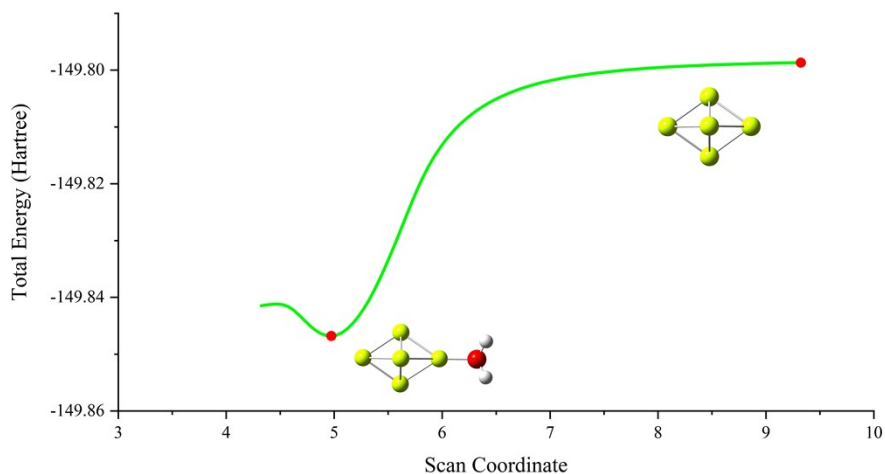


Fig. 1S Flexible scanning of Be₅ clusters with H₂O, the energies are calculated at the PBE0-D3/ Def2TZVP level.

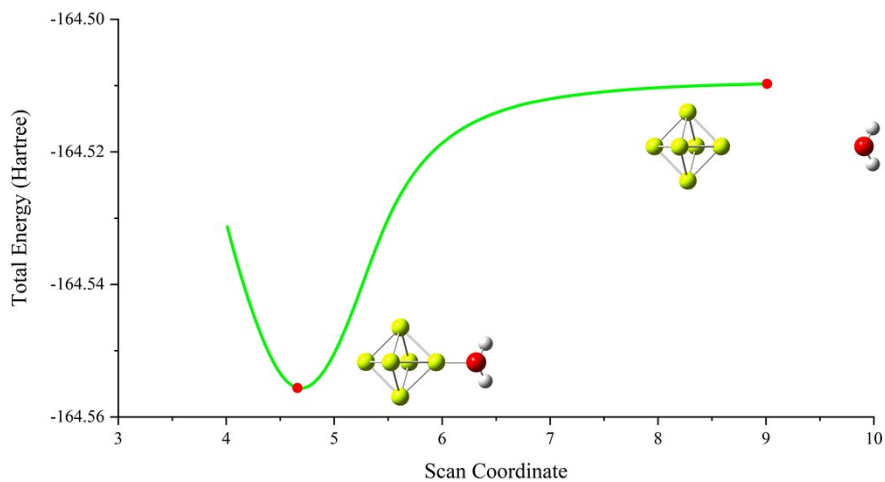


Fig. 2S Flexible scanning of Be₆ clusters with H₂O, the energies are calculated at the PBE0-D3/ Def2TZVP level.

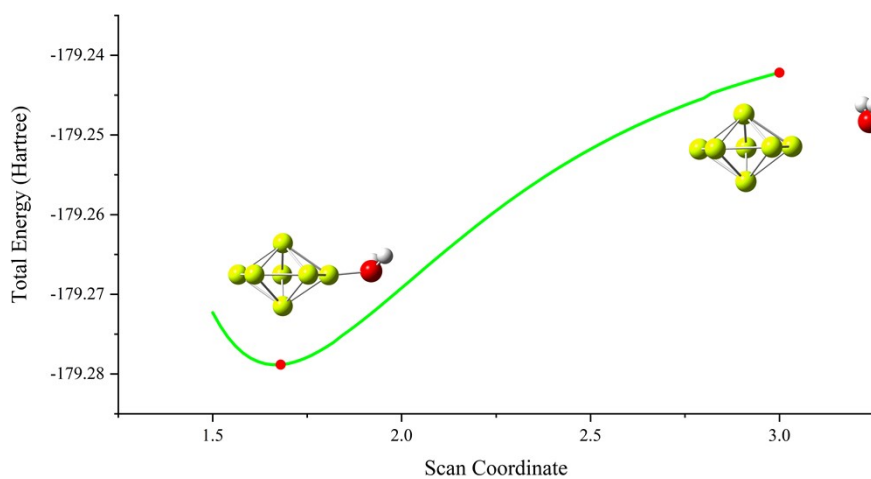


Fig. 3S Flexible scanning of Be₇ clusters with H₂O, the energies are calculated at the PBE0-D3/ Def2TZVP level.

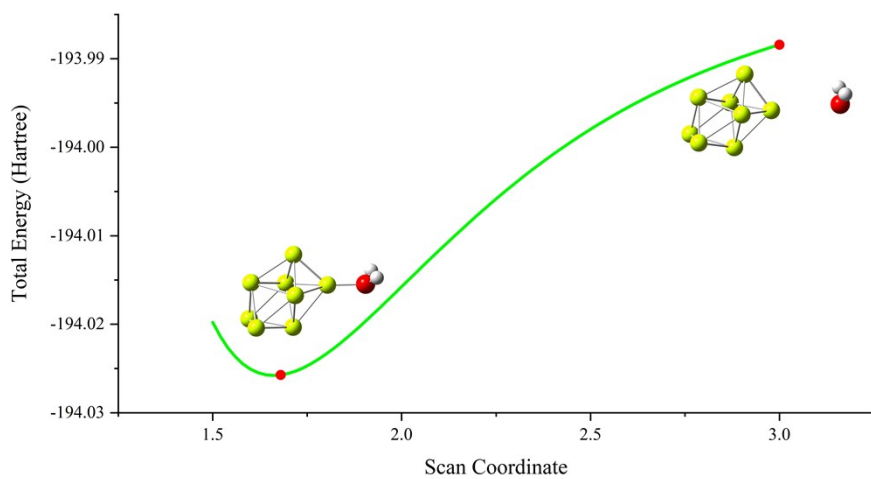


Fig. 4S Flexible scanning of Be₈ clusters with H₂O, the energies are calculated at the PBE0-D3/ Def2TZVP level.

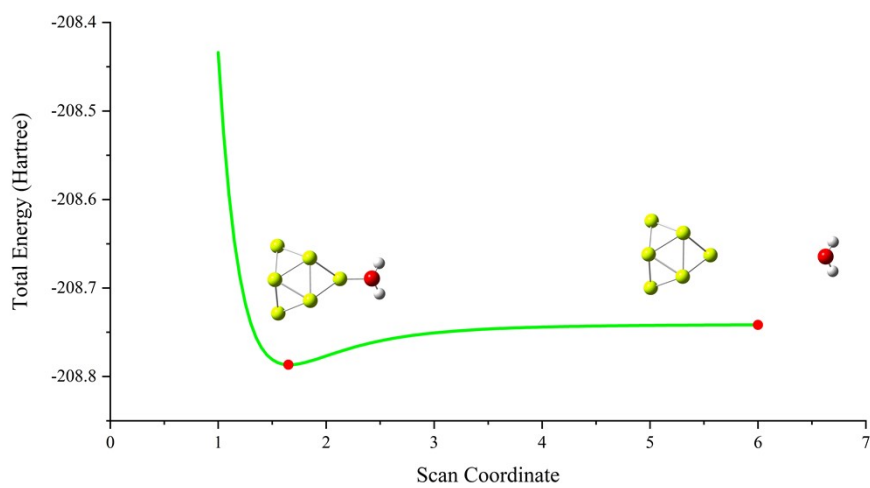


Fig. 5S Flexible scanning of Be₉ clusters with H₂O, the energies are calculated at the PBE0-D3/ Def2TZVP level.