

## Electronic Supplementary Information

### **Stronger-than-Pt hydrogen adsorption in a Au<sub>22</sub> nanocluster for hydrogen evolution reaction**

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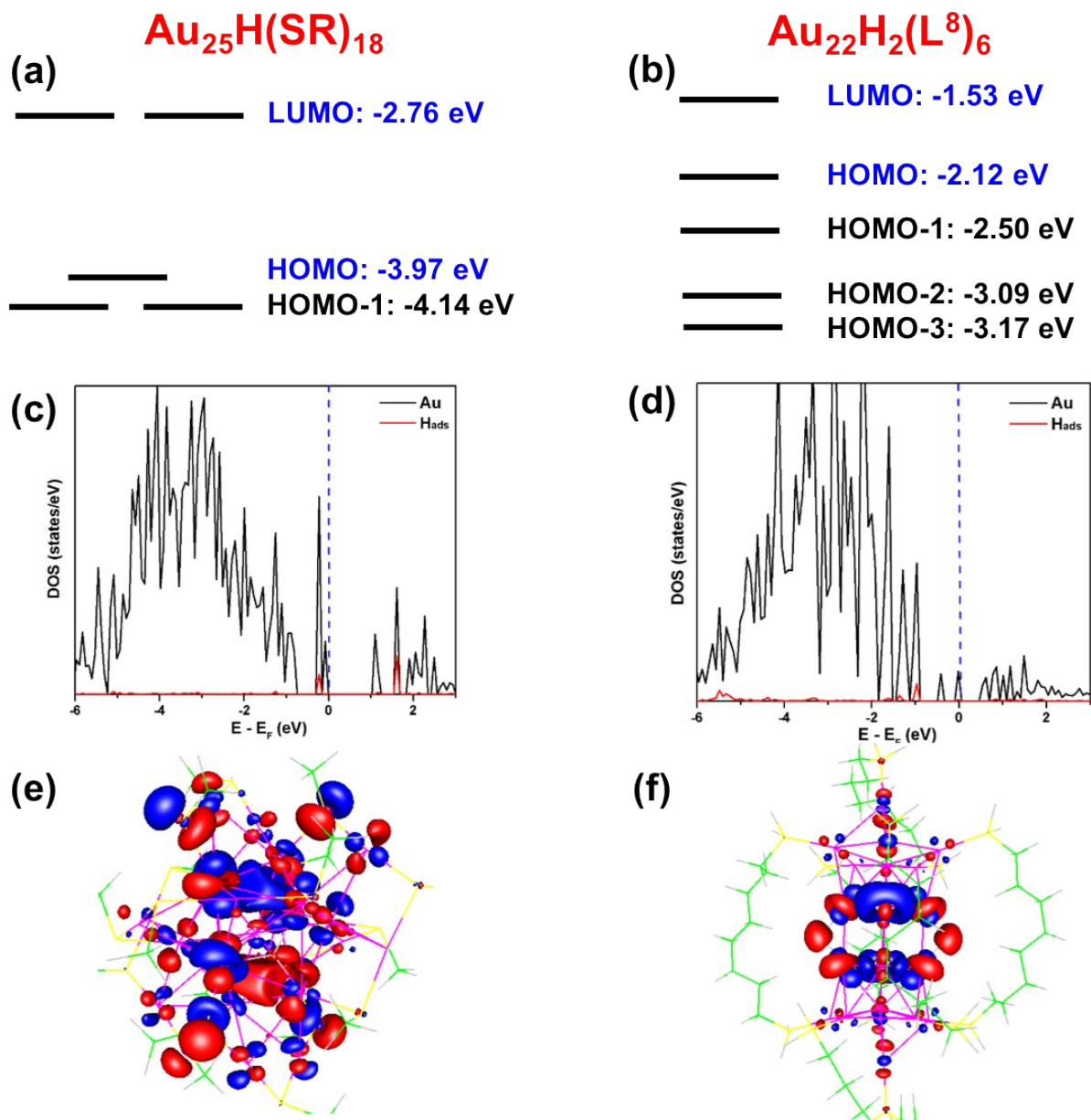


Fig. S1 The eigenvalue spectra of  $\text{Au}_{25}\text{H}(\text{SR})_{18}$  and  $\text{Au}_{22}\text{H}_2(\text{L}^8)_6$  (a and b); the local density of states (DOS) for  $\text{Au}_{25}\text{H}(\text{SR})_{18}$  and  $\text{Au}_{22}\text{H}_2(\text{L}^8)_6$  (c and d) relative to their respective HOMO levels; the HOMO-1 of  $\text{Au}_{25}\text{H}(\text{SR})_{18}$  (e), and the HOMO-2 of  $\text{Au}_{22}\text{H}_2(\text{L}^8)_6$  (f).