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# 从头计算方法比较研究 $B_2Au_4$, $Al_2Au_4$ 和 $BAlAu_4$ 的几何和电子结构

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# A Comparative *Ab initio* Study of the Geometric and Electronic Structures of $B_2Au_4$, $Al_2Au_4$ and $BAlAu_4$

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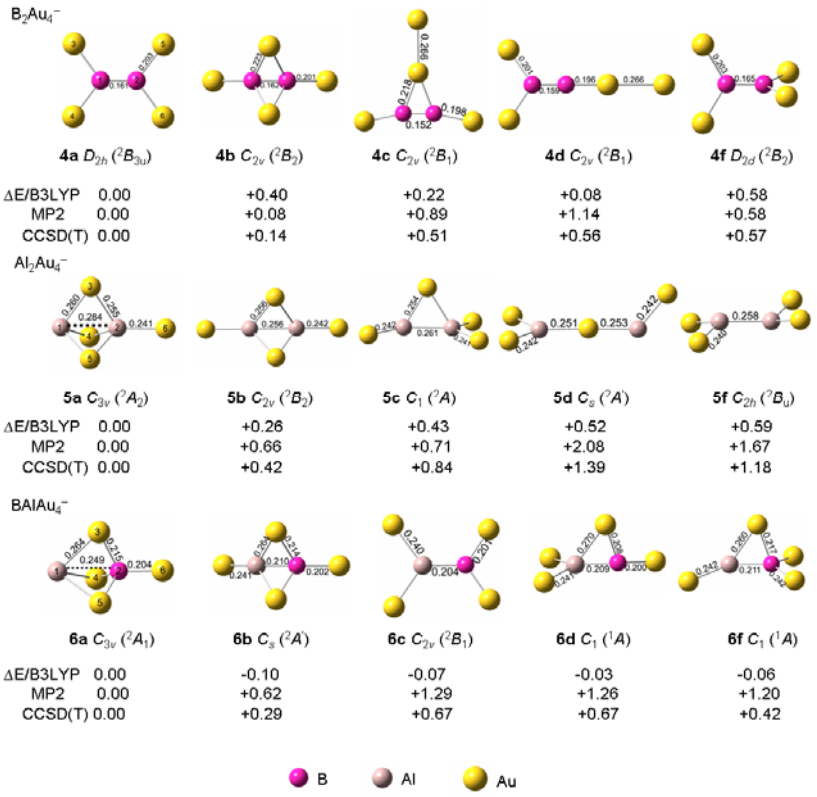


**Fig.S1 Low-lying neutral isomers of $B_2Au_4^-$, $Al_2Au_4^-$ and $BAlAu_4^-$ at B3LYP, with the relative energies Δ*E* (eV) at B3LYP//B3LYP, MP2//MP2, and CCSD(T)//B3LYP indicated**

The bond lengths (in nm) are labeled at B3LYP level.