Supporting Information

Low-energy isomer identification, structural evolution and magnetic properties in manganese-doped gold clusters MnAu\textsubscript{n} (n=1-16)

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Description:

Figure 7. The HOMO and LUMO orbitals of the MnAu\textsubscript{n} (n=1-16) clusters for the lowest-energy structures, yellow indicates that the wave function has a positive sign, while blue indicates a negative sign. The surface isovalue for molecular orbital plotting is 0.03 e/Å\textsuperscript{3}.
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HOMO          LUMO              HOMO               LUMO

MnAu          MnAu$_2$

MnAu$_3$      MnAu$_4$

MnAu$_5$      MnAu$_6$

MnAu$_7$      MnAu$_8$