1. Band structure of Mg$_2$(FeH$_6$) crystal.

Figure S1. Band structure of Mg$_2$(FeH$_6$) crystal. Corresponding first Brillouin zone and the high
symmetry K point paths are shown in the inset: $\Gamma$ (0, 0, 0) $\rightarrow$ X (1/2, 0, 0) $\rightarrow$ M (1/2, 1/2, 0) $\rightarrow$ $\Gamma$
(0, 0, 0) $\rightarrow$ Z (0, 0, 1/2) $\rightarrow$ R (1/2, 0, 1/2) $\rightarrow$ A (1/2, 1/2, 1/2) $\rightarrow$ Z (0, 0, 1/2).
2. Geometric structure of $\text{Mg}_2(\text{FeAu}_6)$ crystal.

**Figure S2.** Structure of $\text{Mg}_2(\text{FeAu}_6)$ crystal. Cyan, green, and yellow atoms are Mg, Fe, and Au, respectively.
3. IR and Raman Spectra of $I_h$ and $O_h$ Isomers of $[\text{Ti@Au}_{12}]^{2-}$.

**Figure S3.** Comparison of IR and Raman spectra between $I_h$ and $O_h$ isomers of $[\text{Ti@Au}_{12}]^{2-}$.
4. Molecular dynamic simulations of Ti@Au\textsubscript{12} and Na\textsubscript{2}[Ti@Au\textsubscript{12}].

![Graph showing energy fluctuations of Ti@Au\textsubscript{12} and Na\textsubscript{2}[Ti@Au\textsubscript{12}]](image)

**Figure S4.** *Ab initio* molecular dynamic simulation showing total energy fluctuations of Ti@Au\textsubscript{12} and Na\textsubscript{2}[Ti@Au\textsubscript{12}] with respect to time at 300 K.
5. Partial density of states of Na$_2$[Ti@Au$_{12}$].

**Figure S5.** PDOS plot of Na$_2$[Ti@Au$_{12}$]-$D_{4h}$. The directions are defined as shown in the inset.
6. Selected isomers of Cs$_2$[Ti@Au$_{12}$] and Mg[Ti@Au$_{12}$].

**Figure S6.** Several low energy isomers of Cs$_2$[Ti@Au$_{12}$] along with their relative energies $\Delta E$ and symmetry point group. The yellow, purple, and light grey spheres represent Au, Cs, and Ti, respectively.

**Figure S7.** Several low energy isomers of Mg[Ti@Au$_{12}$]. The yellow, green, and light grey spheres represent Au, Mg, and Ti, respectively.
7. Molecular Orbitals (HOMO/LUMO) of Cs$_2$[Ti@Au$_{12}$].

![LUMO and HOMO of Cs$_2$[Ti@Au$_{12}$]](image)

Cs$_2$Ti@Au$_{12}$

**Figure S8.** HOMO and LUMO molecular orbitals of Cs$_2$[Ti@Au$_{12}$].