Electronic Supplementary Material (ESI) for Nanoscale.

Superatom Compounds with Internal Electric Fields for Light Harvesting.

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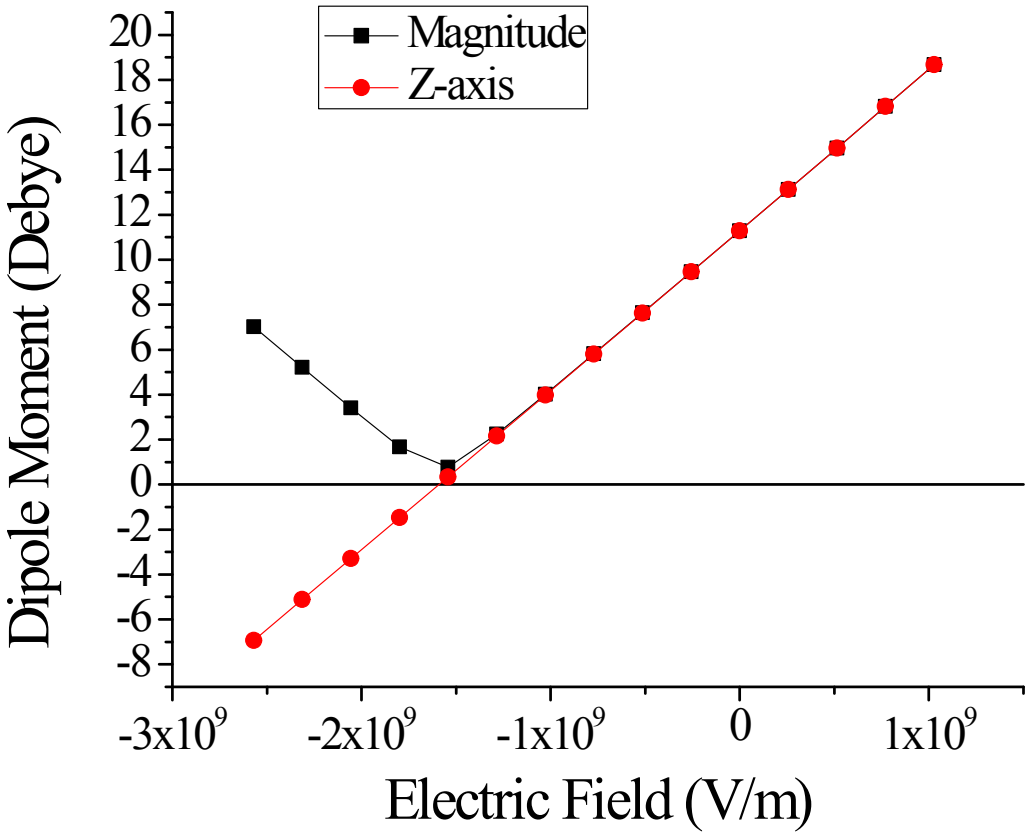

Figure S1. The dipole moment and parallel vector of the dipole moment in $Re_6S_8Cl_2(CO)_3Re_6S_8Cl_2(PMe_3)_3$ as a function of the electronic field strength.

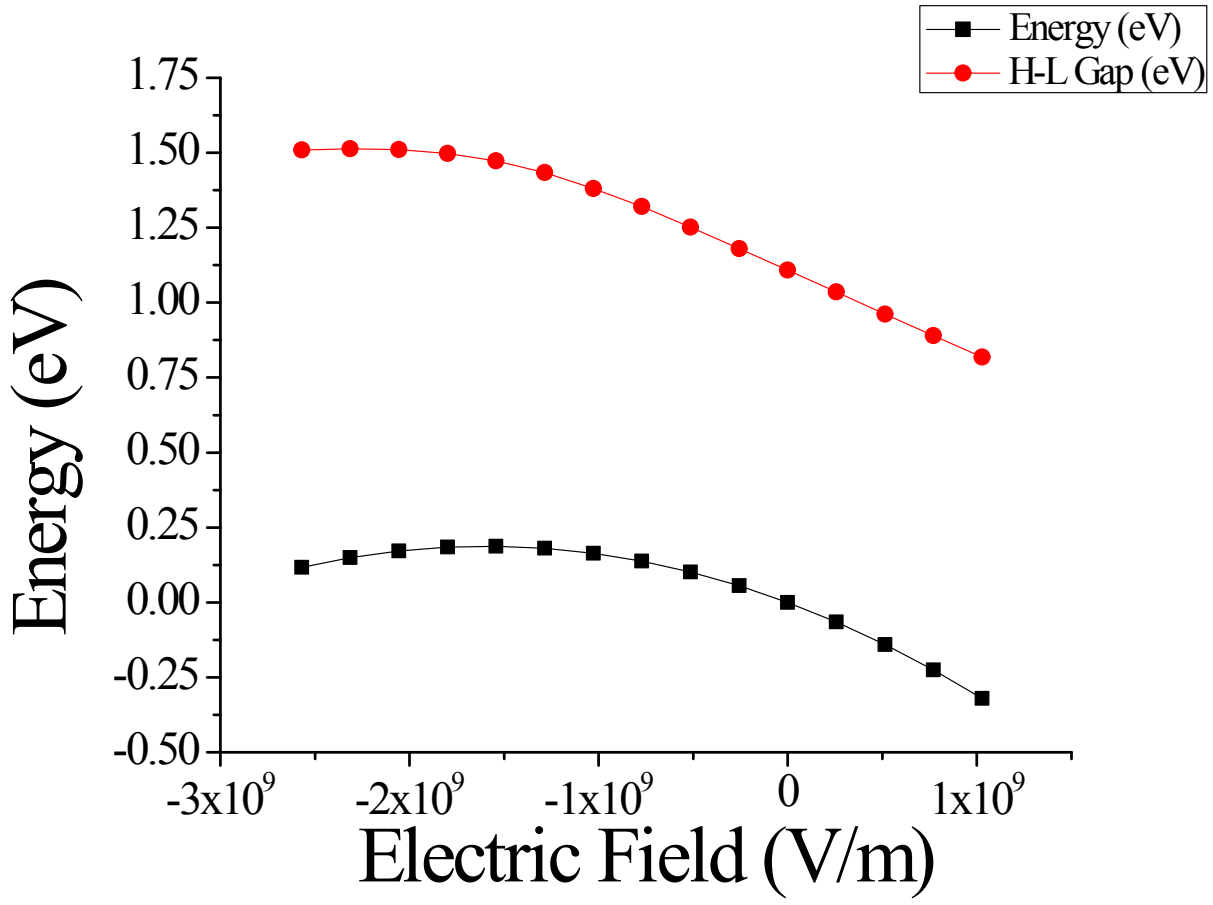

Figure S2. The HOMO-LUMO gap and total energy of $Re_6S_8Cl_2(CO)_3Re_6S_8Cl_2(PMe_3)_3$ as a function of electric field.

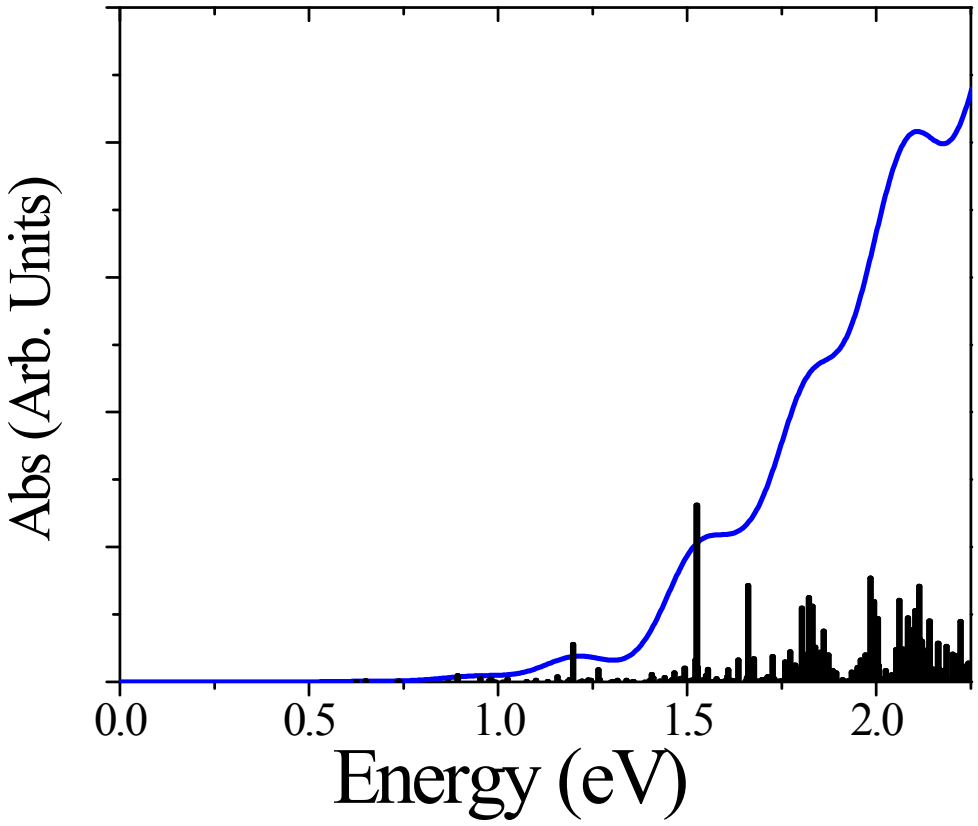

Figure S3. Optical absorption spectra of tetramer $Re_6S_8Cl_2(CO)_3$: $Re_6S_8Cl_2(CO)_2$: $Re_6S_8Cl_2(PMe_3)_2$: $Re_6S_8Cl_2(PMe_3)_3$ cluster.