

Transition Metal Induced Excess Electron Localization Driving Giant First Hyperpolarizability in Alkaline Earthides: A DFT and TD-DFT Study

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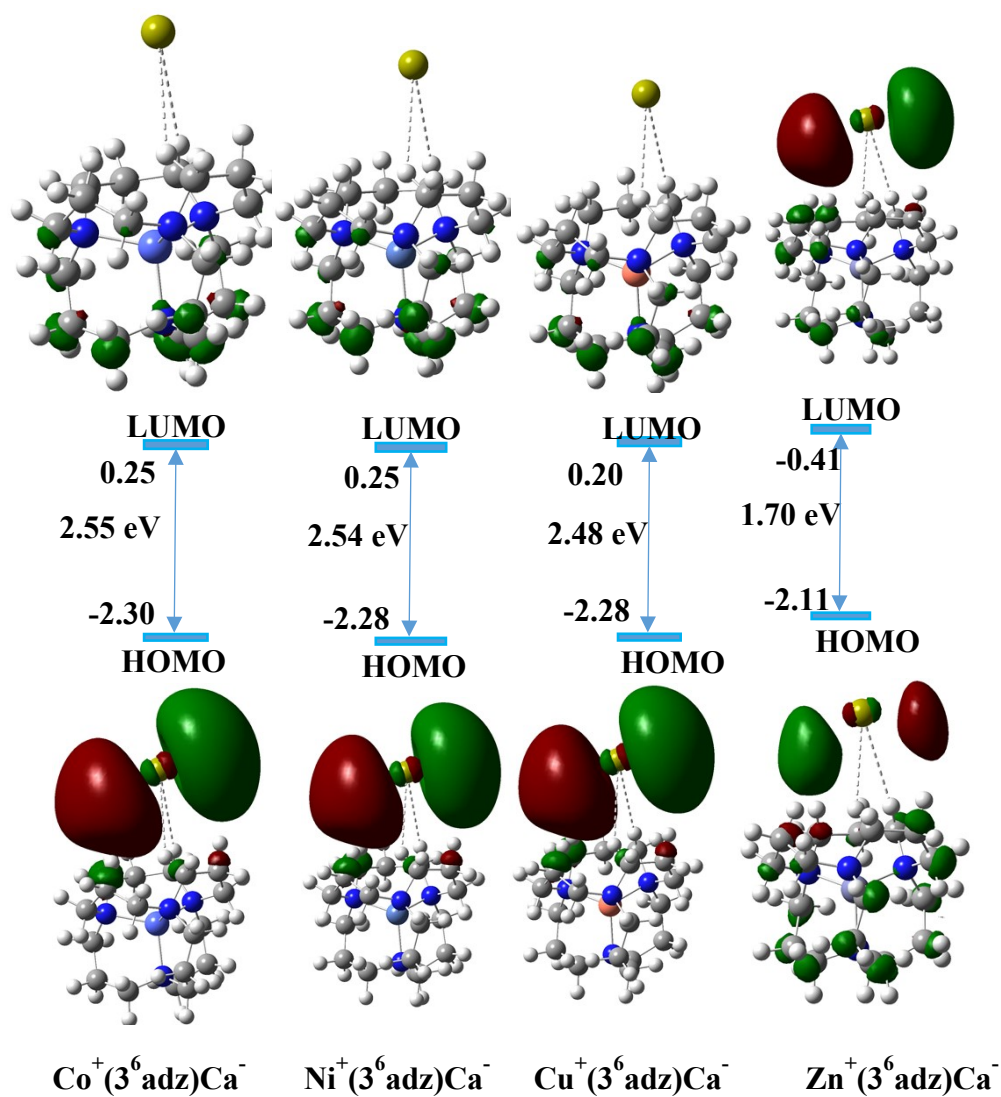
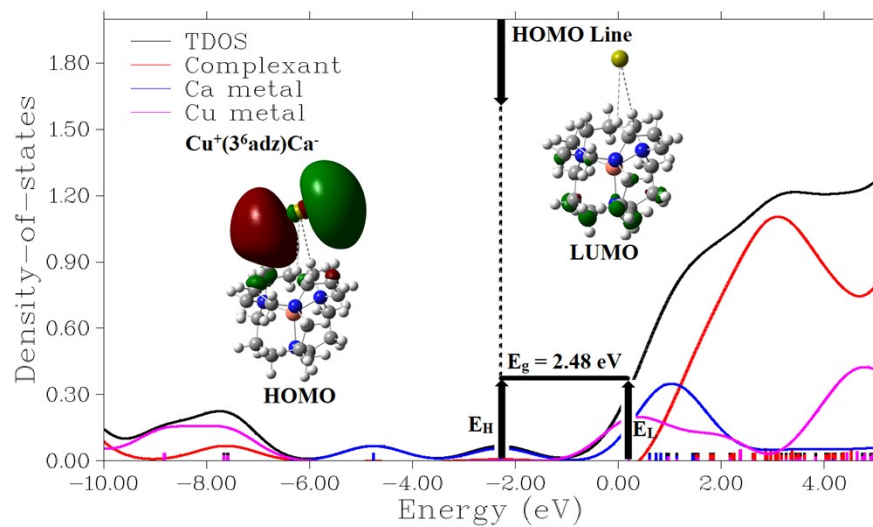
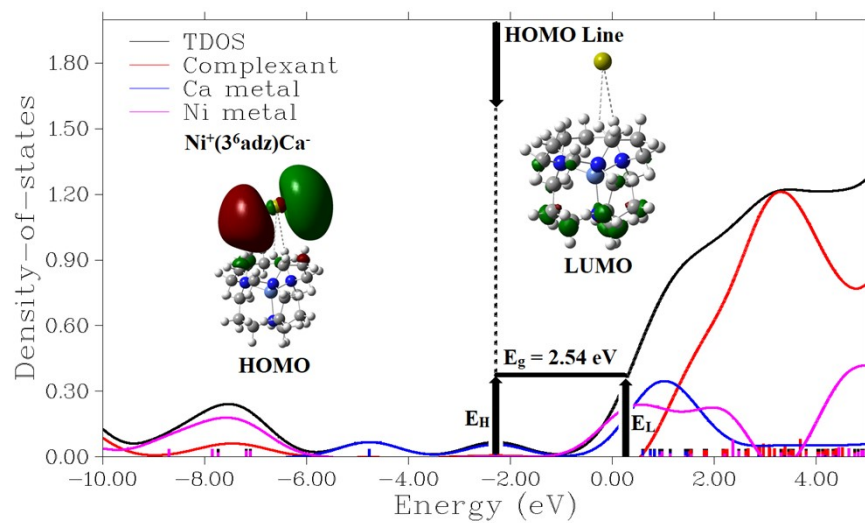
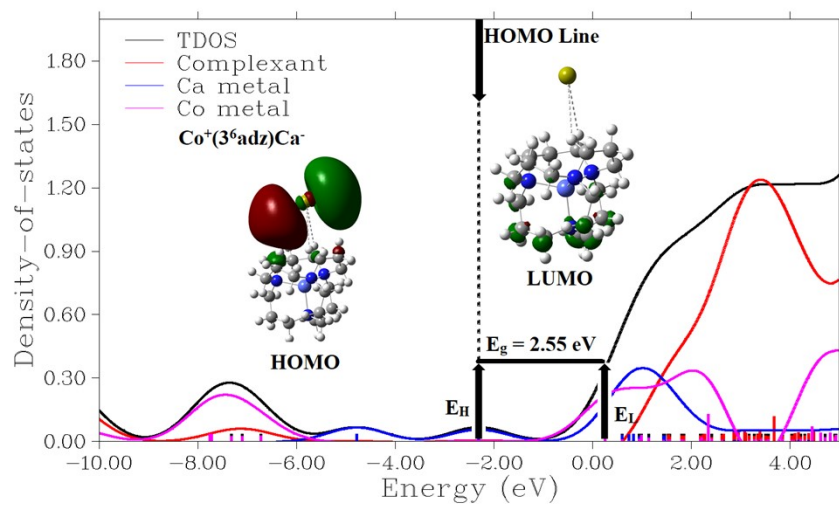


Fig S1. The HOMO and LUMO of $\text{M}^+(3^6\text{adz})\text{Ca}^-$ (here M^+ is Co to Zn) series plotted on iso-value of 0.02.



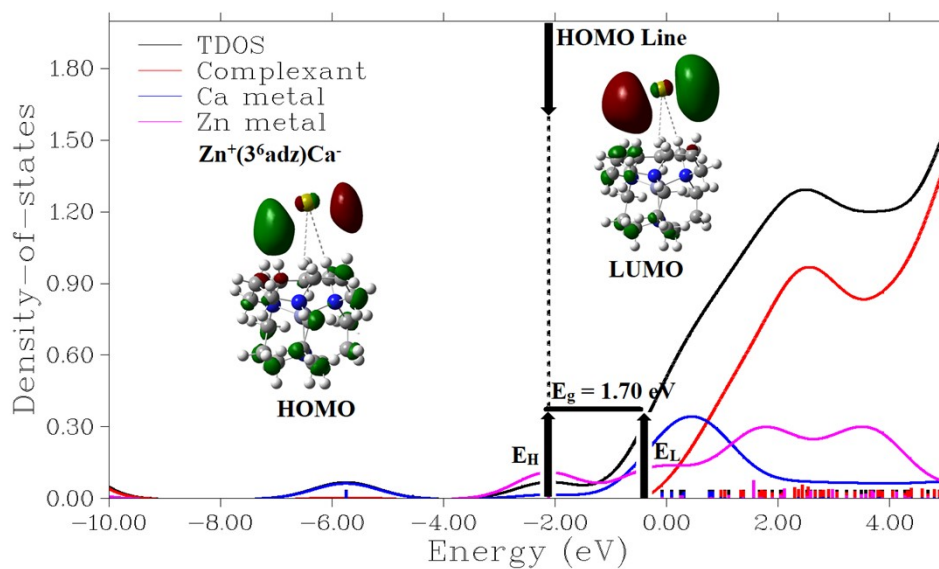
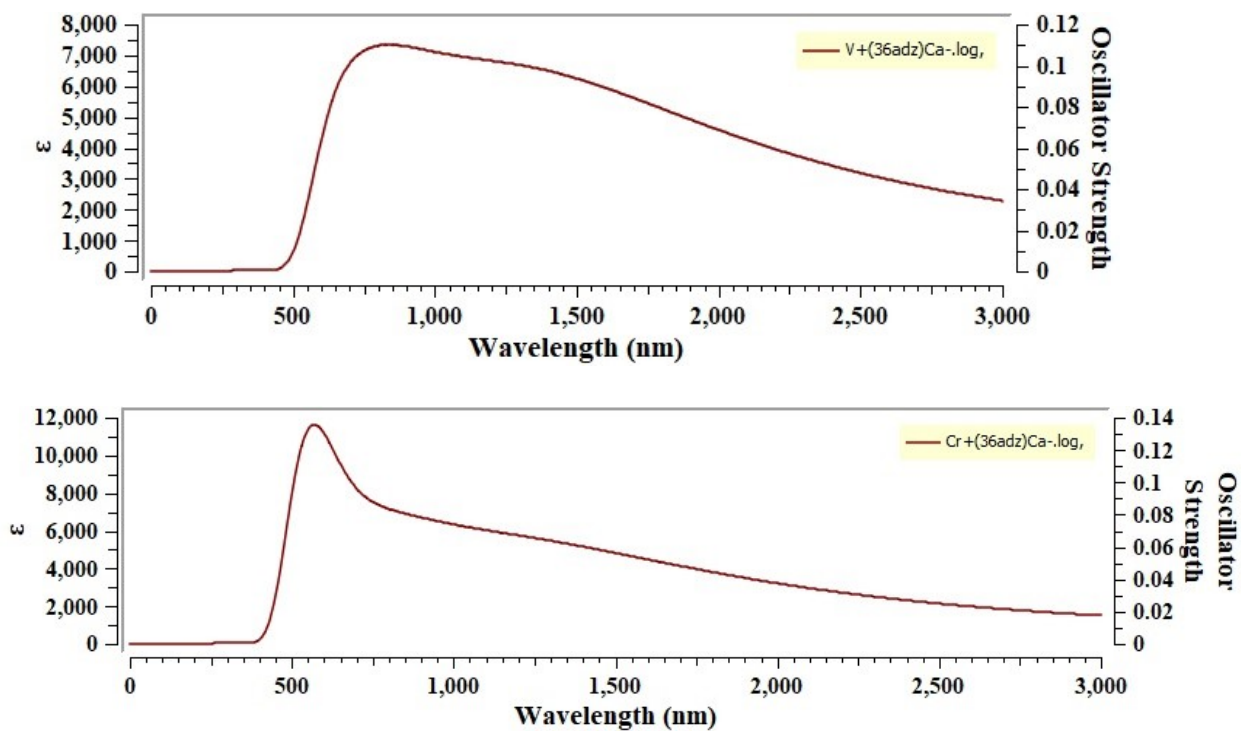
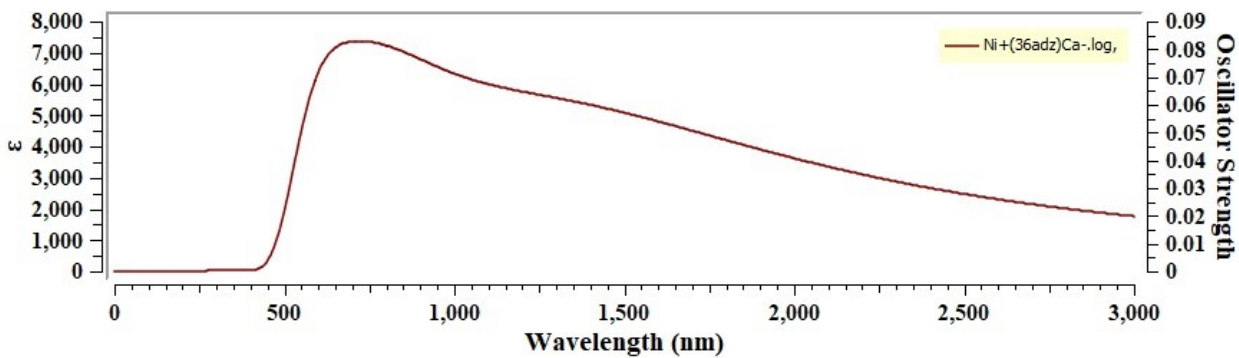
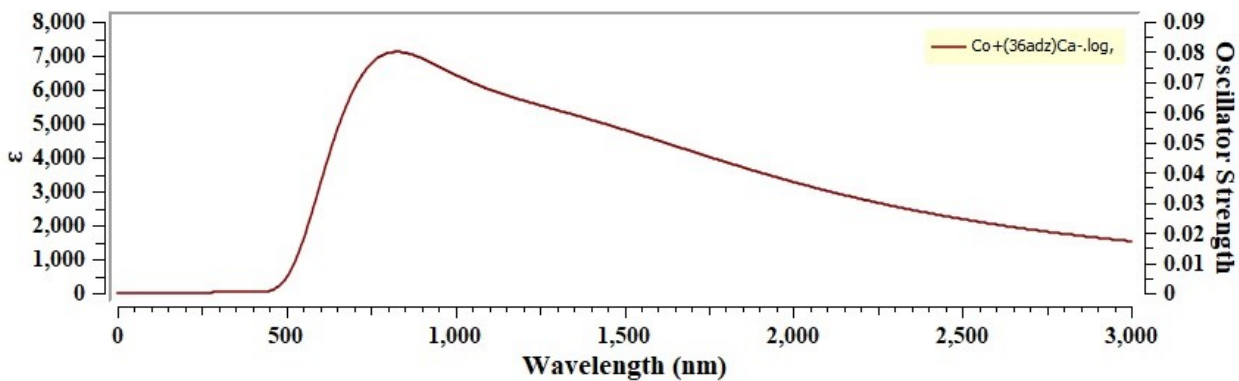
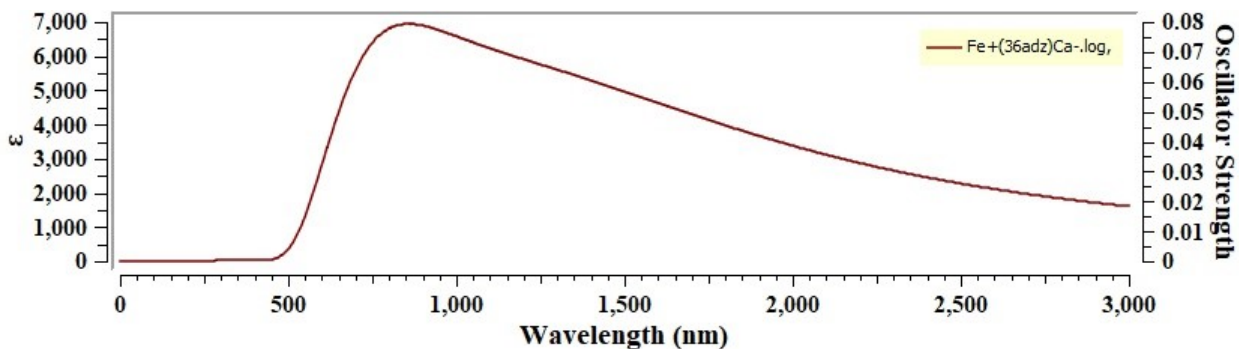
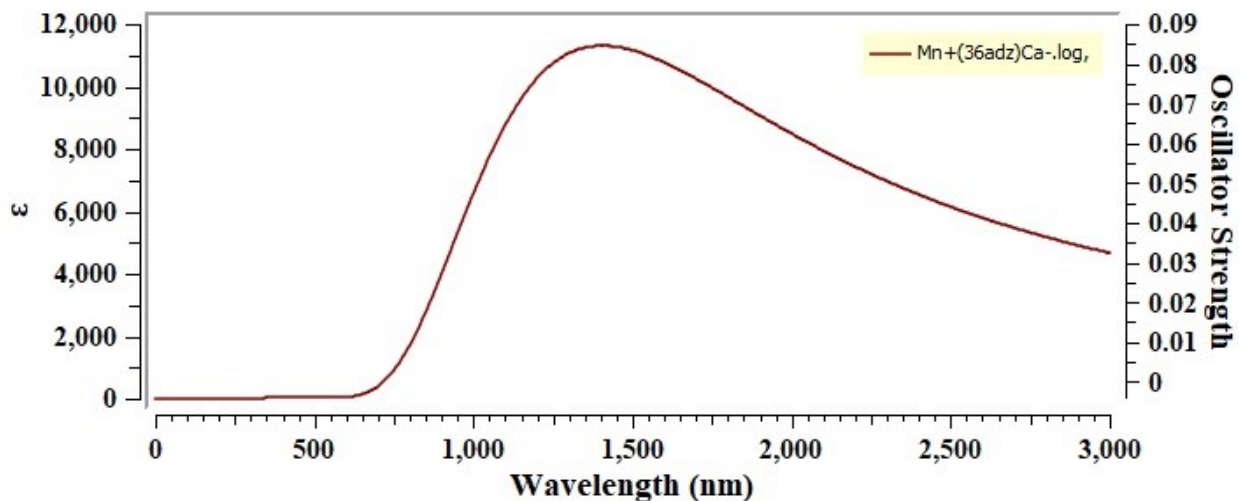


Fig S2. The PDOS spectra of $M^+(3^6\text{adz})\text{Ca}^-$ (here $M^+ = \text{Co}$ to Zn) series generated by using Multiwfn





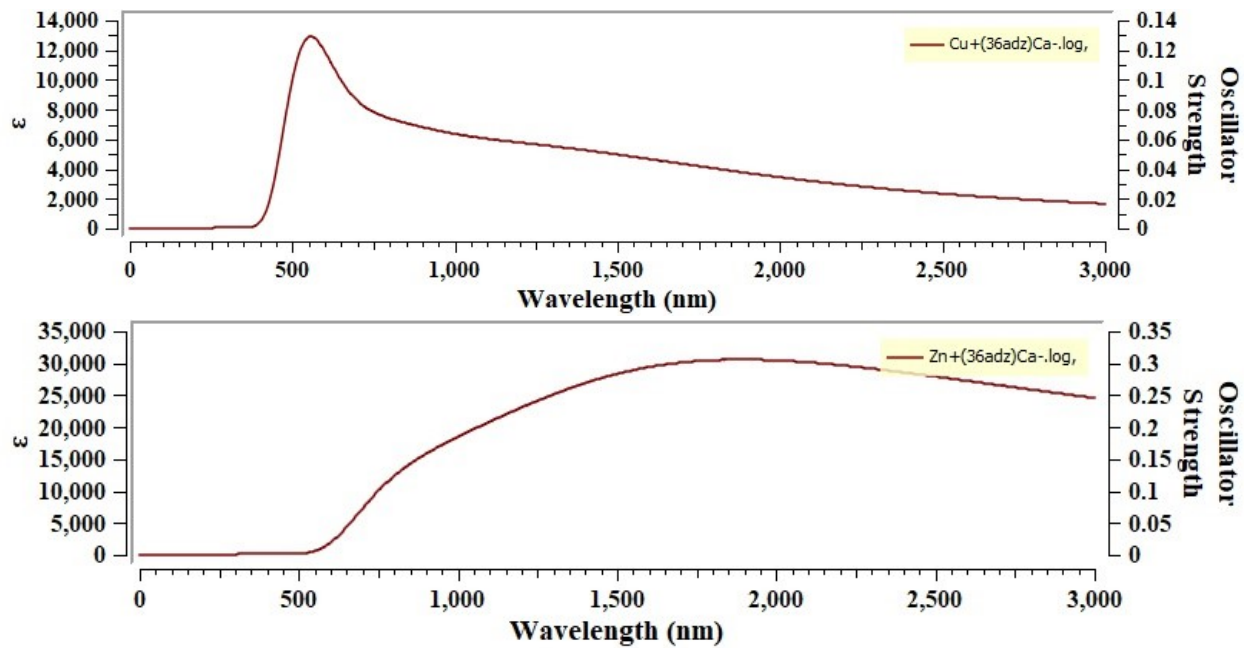


Fig S3. The UV absorption spectra of $M^+(3^6adz)Ca^-$ ($M^+= V$ to Zn) series