Electronic Supplementary Material (ESI) for Nanoscale.


# Supplementary Information

## Tunable Optical Activities in Chiral Transition Metal Oxide Nanoparticles

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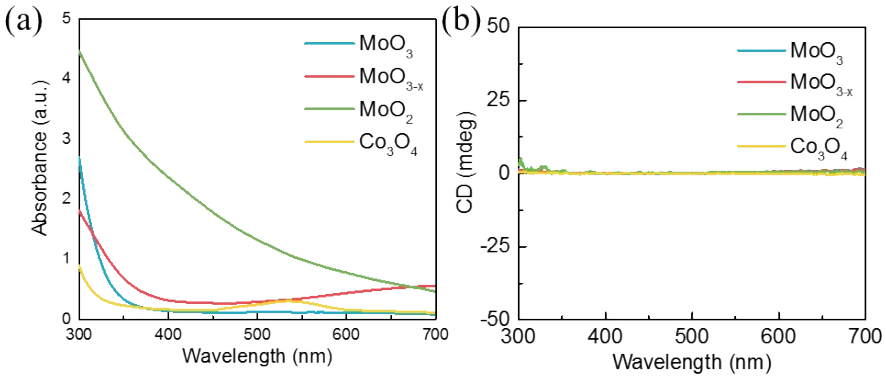


**Figure S1.** a) UV-visible absorption spectra and (b) CD spectra of $MoO_3$, $MoO_{3-x}$, $MoO_2$ and $Co_3O_4$ nanoparticles (NPs) without use of chiral ligands. During the synthesis of $MoO_{3-x}$, $MoO_2$ and $Co_3O_4$ NPs, sodium borohydride was used as a reducing agent.

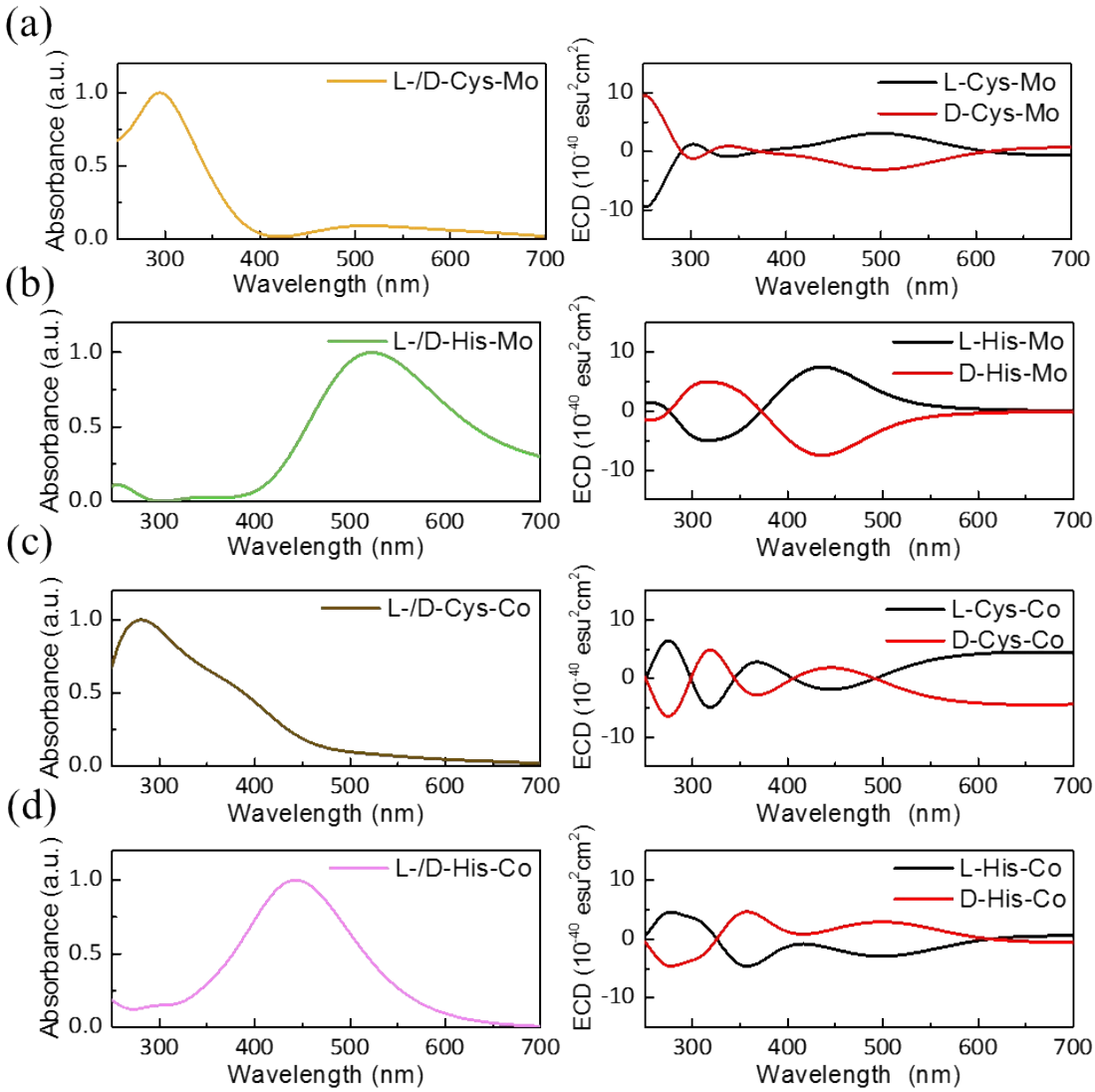


**Figure S2.** The theoretically calculated UV-vis absorption spectra (Left column) and ECD (Right column) using TD-DFT for (a) L-/D-Cys-Mo, (b) L-/D-His-Mo, (c) L-/D-Cys-Co and (d) L-/D-His-Co in zwitterionic state.

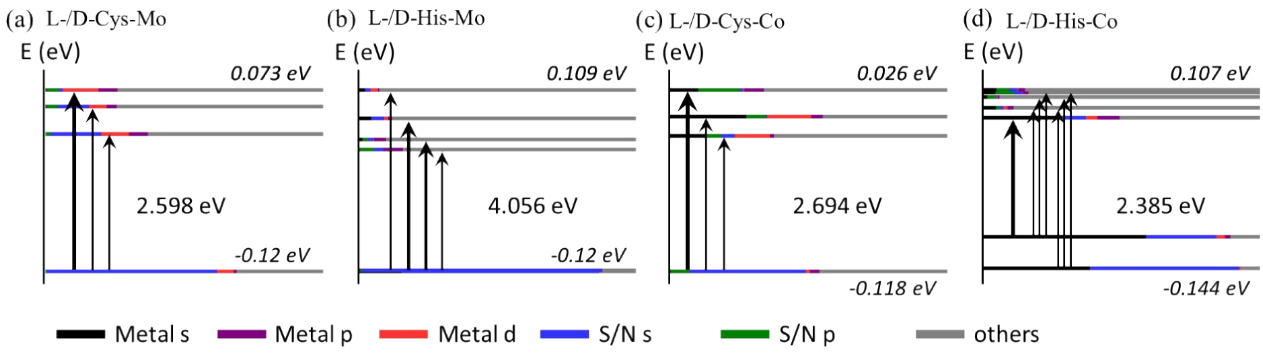


**Figure S3.** The electronic transitions of (a) L-/D-Cys-Mo; (b) L-/D-His-Mo; (c) L-/D-Cys-Co and (d) L-/D-His-Co. The metal represents Mo or Co atom. S/N represents S atom in cysteine and N atom in histidine, and both of them are connected directly to the metal atoms.

In Figure S3, the involved orbitals are lined up according to the eigenvalues, i.e. energy. The different colors represent different molecular orbitals. Black, purple and red colors represent the s, p, and d orbitals of the metal atoms. Blue and green colors represent the s and p orbitals of the atoms that connect the ligand molecules and metal atoms. Gray color represent other orbitals of ligand molecules. The transition at the same wavelength is contributed by different orbital transitions. The thickness of the arrow represents the probability that the transition will occur.

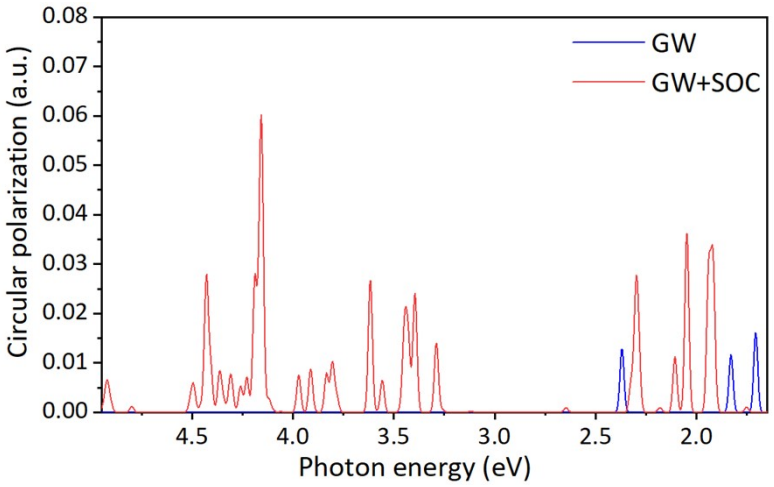


**Figure S4.** The theoretically calculated circular polarization spectrum of D-Cys-Co using GW approximation and GW+SOC methods, respectively. The x-axis (photon energy) is adjusted to match the wavelengths in CD spectra.

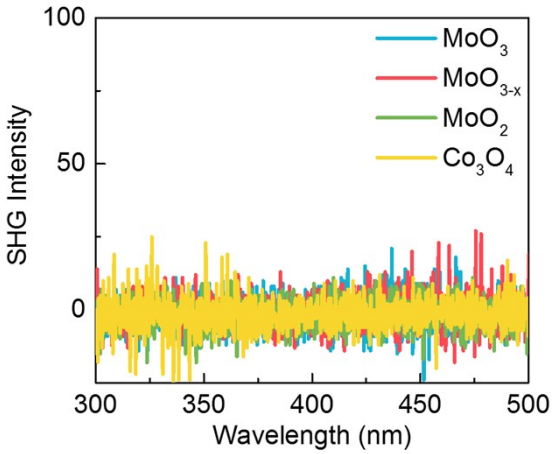


**Figure S5.** SHG signals of achiral $MoO_3$, $MoO_{3-x}$, $MoO_2$ and $Co_3O_4$ NPs excited at 800 nm.