

# Induced Chirality in Halide Perovskite Clusters through Surface Chemistry

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## ABSTRACT

The chiroptical properties of materials are of interest for various applications, including structure determination, polarized photo-detectors/luminescence sources, and spintronics. Inducing chiroptical activity into semiconductor materials presents a challenge due to the difficulty of controllably creating asymmetric crystal structures. One promising method is to use chirality transfer by deploying chiral organic molecules as capping ligands for nanocrystals. Experimentally, chiral capped nanocrystals show emergent chiroptical signatures, but the mechanisms for chirality transfer remain unclear. Here we utilize atomistic modeling using time-dependent density functional theory calculations to explore chirality transfer in CsPbX<sub>3</sub> (X=Cl, I) clusters that are capped with chiral diaminocyclohexane (DACH) enantiomers. When DACH enantiomers are bound to the cluster surface, chirality transfer is observed. Namely, perovskite optical transitions gain chiroptical activity that is dependent on the binding configuration. We find that this chirality transfer is best rationalized by the coupling of the static dipoles from the surface adsorbed chiral molecules to the optical transition dipole of the perovskite cluster. The ratio of circular dichroism (CD) to absorption, known as the anisotropy factor ( $g$ ), is found to increase proportionally to surface ligand density and provides mechanistic insight for improving the chiroptical functionality of semiconductor nanomaterials.