Materials theory of halide perovskites

Abstract: Halide perovskites have gained prominence in optoelectronics and quantum materials due to their chemical versatility, which allows for a broad range of interactions with light, electrons, spins, and lattice vibrations. My team employs first-principles methods like density functional theory, tight-binding models, and machine learning-accelerated molecular dynamics to explore their complex structure-property relationships. We focus on defect chemistry to enhance solar cell efficiency and stability, identifying and mitigating defects that cause losses and degradation through compositional adjustments and surface treatments. Additionally, we explore the chirality of perovskites, using chiral ligands to introduce properties like chiral-induced spin selectivity and enhancing chiral optical activity. This exploration aims to harness these distinctive properties for pioneering applications in spin LEDs and chiral photodetectors, driven by a deep understanding of the relation between structural features and optoelectronic properties.

Shuxia Tao