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First Principle Hybrid Density Functional Theory Study of Halide Perovskite Surfaces and Interfaces ERIC WELCH, ALEX ZAKHIDOV, Texas State University — Perovskite materials continue to revolutionize multiple optoelectronic fields with applications in solar cells, light emitting diodes, photodetectors and lasers. High quality devices are developed with low-cost precursors at room temperature using solution processing. Computational studies have been used to predict new perovskites and transport layer interfaces as well as describe the photophysics of already-made devices so perovskite-based technologies can reach their full potential. We show here hybrid density functional theory calculation on the interface between an inorganic perovskite ($CsPbBr_3$) and inorganic hole transport layer (CuI). Band offset calculations between $CsPbBr_3$ and CuI reveal the tunability of the interface offset potential through varied material thickness, where the offset converges for structures over nine-unit cells thick. Experiments have recently been published showing the viability of CuI as a hole transport layer in perovskite-based devices.

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