Advancements in $CsPbI_3$ Inorganic Perovskite Solar Cells: Role of Selective Transport Layers and Insights from Density Functional Theory

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Abstract

In recent years, $CsPbI_3$ perovskite has garnered significant attention due to its excellent thermal stability and ideal bandgap, making it an excellent choice for tandem silicon-perovskite solar cells (PSCs). However, the current fabrication processes for single-junction $CsPbI_3$ PSCs are incompatible with underlying silicon heterojunction (Si-HJ) solar cells, primarily due to the high temperatures required for the deposition of the TiO_2 layer as the electron transport layer (ETL).
This talk will explore alternative ETL materials to replace TiO_2 and strategies to enhance the interface between these materials and the $CsPbI_3$ perovskite. Additionally, it will demonstrate how density functional theory (DFT) simulations can provide atomistic insights that help interpret experimental findings, offering a deeper understanding of the system.