Design and Optimizaiton of Degital-Twins of Perovskite Solar Cells

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Computer simulation using a solar-cell device simulator and machine learning methods are applied in order to design and discover optimal device structures and materials for the development of perovskite solar cells. In the presentation, we will show optimal layer thickness and electronic-structure-related parameters in metal-halide perovskite solar cells. A strategy to design realistic material using the first-principle calculation will be discussed.