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Engineering Strategies for Perovskites: From DFT to Machine Learning

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The depletion of fossil fuels and rapid growth in world population are the main drivers of research interests to find alternative renewable energy sources that could alleviate the global energy crisis. Hence, perovskite solar cells have been largely explored as a prospective source of clean and renewable energy. They have shown remarkable progress with rapid increases in power conversion efficiency, from early reports of approximately 3% in 2009 to over 25% today. Despite their excellent optoelectronic characteristics such as tuneable band gap, high absorption coefficients, high carrier mobility, and long diffusion lengths for electrons and holes, small effective masses and facile fabrication; they still have a number of drawbacks that hinder their practical application and commercialisation. Perovskite solar cell devices must retain high efficiencies while exhibiting decent stability and acceptable degradation for practical applications. Herein, using first-principle approach we explore different engineering strategies for various perovskites materials, namely, all-inorganic halide perovskites, organic-inorganic perovskites and double perovskites crystal structures and their respective optoelectronic characteristics. In addition, data-driven machine learning approach is used to conduct compositional space exploration to discover new perovskite materials.

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