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Machine Learning (ML)-Assisted Fabrication and Scattering data for Solar Cells

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Research on Machine Learning(ML) for Organic Solar Cells (OSCs) has currently tremendously increased. The performance of OSCs specifically depends on solvents, crystallinity, molecular orientation of absorbing layer, and morphology of active and interfacial layers. The complex nature of organics is demanding more efficient and eco-economic, and eco-friendly ML models such as photovoltaic phenomena are related to microscopic properties and require high-accuracy quantum calculations. For high accuracy, large-scale virtual screening is required, but on the other hand, high computational cost made it difficult for large-scale virtual screening. When a researcher fabricates a novel device from a novel material system, it often takes many weeks of experimental effort and data analysis to understand why any given device/material combination produces an efficient or poorly optimized cell. Here, we combine machine learning, device modelling and experimentation to effectively optimize the OPV fabrication process. ML techniques can effectively model the correlation between the properties of the OPV materials and the corresponding fabrication methods if they are trained using sufficient experimental data. Moreover, we highlight the integration of machine learning methods into the typical workflow of scattering experiments. We focus on scattering problems that faced challenge with traditional methods but addressable using machine learning, such as leveraging the knowledge of simple materials to model more complicated systems, learning with limited data or incomplete labels, identifying meaningful spectra and materials'representations for learning tasks, mitigating spectral noise, and many others.

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