Machine Learning For Materials And Device Simulations

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I will describe the application of machine learning methods in a new context. Specifically, how we address a scientific question that enables comparison between physics-based simulation and measurements in a way that can straightforwardly be generalized. Our method allows for uncertainty in the model input parameters, an area rarely discussed in materials modelling.

In this talk I will demonstrate a novel use of Bayesian Optimisation to relate simulation model results to experimental measurements on charge-carrier dynamics in the lead halide perovskite semiconductor methyl-ammonium lead iodide $MAPbI_3$. Halide perovskite solar cells are highly topical as they have rapidly emerged as leading contenders in photovoltaic technology. We show how Bayesian Optimisation can efficiently search the model input space of a simulation to minimise the difference between the simulation output and a set of experimental results. This method also allows an explicit evaluation of the probability that the simulation can reproduce the measured experimental results in the region of input space defined by the uncertainty in each input parameter. I will show how mesoscale simulation models of charge transport in lead halide perovskites, using an ensemble Monte Carlo approach based on Boltzmann transport theory, can provide insight into mobility-limiting mechanisms. Figure 1 [1] demonstrates how the method can also quantify the effective importance (the "inverse length-scales" of the figure) of each input parameter in determining the simulation outcomes.

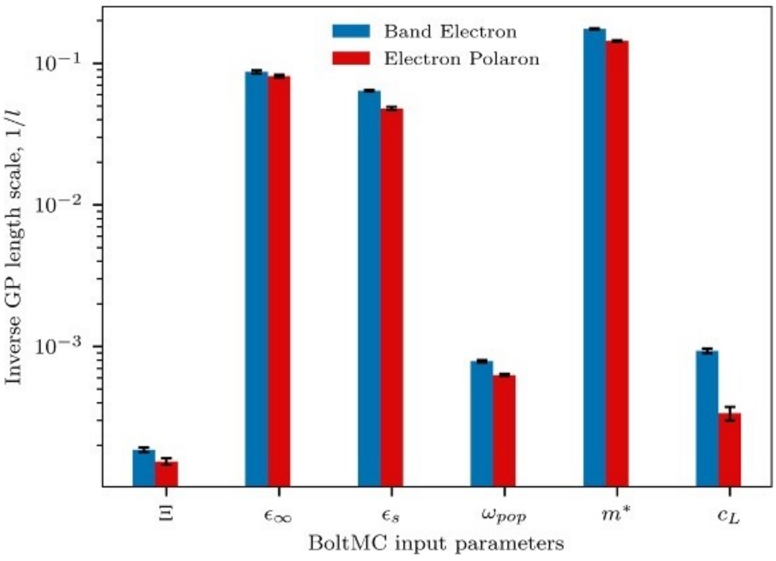

Figure 1. Inverse length-scales of the covariance function for each simulation input parameter, plotted such that larger values indicate larger output (mobility) sensitivity to that parameter. Error bars show standard error in the mean in black. Ξ is the acoustic deformation potential, ε_∞ (ε_s) the high (low) frequency permittivity, ω_{pop} the polar optical phonon frequency, *m** the effective mass and c_L the elastic constant.

1. S. G. McCallum, J. E. Lerpiniére, K O Jensen, P. Friederich, A. B. Walker APL Machine Learning (2023) in review