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Multifidelity Learning Models for Accurate Bandgap Predictions of Solids TURAB LOOKMAN, GHANSHYAM PILANIA, JAMES E. GUBERNATIS, Los Alamos National Laboratory — We present a multidelity co-kriging statistical learning framework that combines variable-fidelity quantum mechanical calculations of bandgaps to generate a machine-learned model that enables low-cost accurate predictions of the bandgaps at the highest fidelity level. In addition, the adopted Gaussian process regression formulation allows us to predict the underlying uncertainties as a measure of our confidence in the predictions. Using a set of 600 Elpasolite compounds as an example dataset and using semi-local and hybrid exchange correlation functionals within density functional theory as two levels of modelities, we demonstrate the excellent learning performance of the method against actual high fidelity quantum mechanical calculations of the bandgaps. The presented statistical learning method is not restricted to bandgaps or electronic structure methods and extends the utility of high throughput property predictions in a significant way.

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