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Machine Learning methods in fitting first-principles total energies for substitutionally disordered solid[1] QIN GAO, SANXI YAO, MICHAEL WIDOM, Carnegie Mellon University — Density functional theory (DFT) provides an accurate and first-principles description of solid structures and total energies. However, it is highly time-consuming to calculate structures with hundreds of atoms in the unit cell and almost not possible to calculate thousands of atoms. We apply and adapt machine learning algorithms, including compressive sensing, support vector regression and artificial neural networks to fit the DFT total energies of substitutionally disordered boron carbide. The nonparametric kernel method is also included in our models. Our fitted total energy model reproduces the DFT energies with prediction error of around 1 meV/atom. The assumptions of these machine learning models and applications of the fitted total energies will also be discussed.

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