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Including crystal structure attributes in machine learning models of formation energies via Voronoi tessellations.

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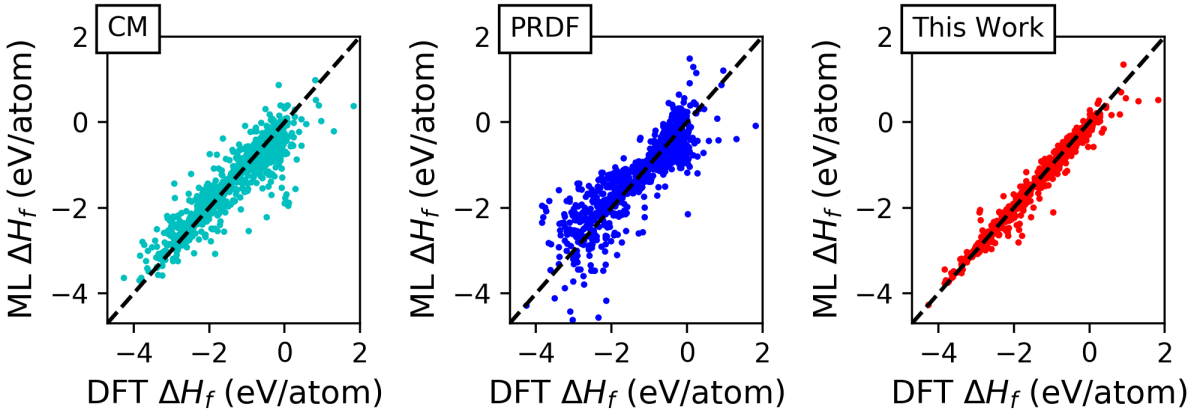

R:	0.923	R:	0.858	R:	0.988
MAE:	0.25 eV/atom	MAE:	0.37 eV/atom	MAE:	0.09 eV/atom
RMSE:	0.38 eV/atom	RMSE:	0.50 eV/atom	RMSE:	0.15 eV/atom
Max Error:	2.03 eV/atom	Max Error:	2.21 eV/atom	Max Error:	1.30 eV/atom

Caption: *This figure compares the performance of three machine learning techniques that predict the properties of a material given its crystal structure: the Coulomb Matrix (CM), Partial Radial Distribution Function (PRDF), and the Voronoi-based ML method described in this report. Each model was trained using same set of 30000 entries from the OQMD, and the above plots show the performance of this model on the same validation set of 1000 compounds from the OQMD. Our technique performs better by every metric.*

Scientific Achievement

In this work, we developed a new approach for building machine learning models that take the crystal structure of a material as input. Our method works by extracting information about the local environment around each atom (e.g., how many neighbors it has) based on the Voronoi tessellation the crystal structure. In this study, we show that our method achieves better accuracy and scales to larger datasets than other machine learning methods proposed for linking crystal structures and their properties.

Significance

Our new method improves our ability to discover new crystalline materials. First of all, the improvement in accuracy over existing methods leads to better predictions of new materials.

Secondly, the improvements in training time let us use all 400,000+ entries in the OQMD as a training set, which further increasing the accuracy of our models. Both of these features have allowed us to discover new Quaternary Heusler materials, and we have made the software for using these models so that others can employ them for materials discovery.

Citation

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