

Composition-based oxidation states and densities of states from physically inspired machine learning

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Oxidation states are widely used in materials chemistry to guide synthesis, understand atomic structure, and predict properties. I will present a machine learning approach that is physics-based and interpretable for predicting oxidation states directly from composition. The interpretability of the results makes them a valuable tool to guide materials chemistry. The resulting predictions can be used to rapidly screen materials and predict atomic structure. I will further present the results of a related machine learning algorithm that can be used to rapidly estimate densities of states directly from composition. I will discuss the limitations, future extensions, and potential applications of both of these tools.