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"Graph Networks as a Universal Machine Learning Framework for Molecules and Crystals."

Abstract: Fast, accurate and transferable surrogate models for property prediction have the potential to rapidly accelerate materials design and discovery. However, classical machine learning models typically depend on feature engineering and the transferability is limited in vast chemical space. Graph networks are a new ML paradigm that supports both relational reasoning and combinatorial generalization. Graphs are a natural representation for a system of atoms and the bonds between them. In addition, graph networks employ graph-level attributes to include structural independent states. Here, we develop, for the first time, MatErials Graph Network (MEGNet) for accurate property predictions in molecular and crystalline materials. We show that the MEGNet models outperform existing ML models in 11 out of 13 properties of the QM9 molecule data set. Furthermore, a single-task MEGNet model can accurately predict internal energy, enthalpy and free energy using temperature, pressure and entropy as graph-level inputs. Similarly, the MEGNet models trained on ~60, 000 crystalline materials achieved significantly lower errors compared to the state-of-the-art models on formation energy, band gap and elastic moduli. Such MEGNet models are interpretable and well-known chemical trends of elements can be extracted from the model-learnt elemental embeddings. Lastly, we demonstrate that transfer learning of elemental embeddings trained from a larger data set can accelerate the training of property models with smaller amounts of data, addressing one of the critical bottlenecks to application of machine learning in materials science.