Chemically-Inspired Bonding Features in MEGNet Enhance Materials Properties Predictions

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Abstract

Over the past decade, machine learning (ML) and graph neural networks (GNN) have demonstrated great success in predicting materials properties. Those ML and GNN models utilized elemental and structural features but not many GNN models utilized chemically inspired bonding features. In this work, we add chemical bonding features such as integrated crystal orbital Hamilton populations (ICOHP) and integrated crystal orbital bond index (ICOBI) from LOBSTER software [1-6]. Such bonding features were utilized to screen new materials and in ML models in previous works [7-8]. Those chemical bonding features are added as edge features in the graphs to encode bonds strength and covalency messages using the values of ICOHP and ICOBI, respectively, which will improve the graphical representation of materials. We add those chemical bonding features computed by Refs. [9-10] to the graph convolution layer of MEGNet [11] to update the edges, nodes, and state features. We anticipate that the modified MEGNet model to improve materials properties predictions such as last phonon peak frequency, bulk modulus, shear modulus, and formation energy per atom [9-10].

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Figures

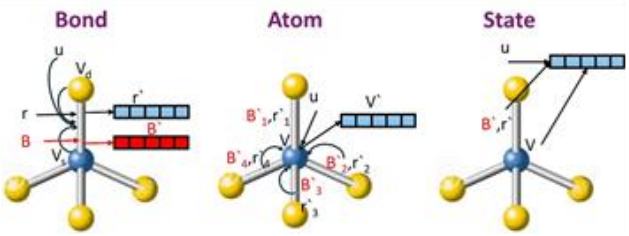

Figure 1. Schematic Figure 1 of MEGNet After adding ICOHP or ICOBI edge features. The symbols represent: “B”: ICOHP or ICOBI edge features, “r”: bond length features, “V”: node features, u: state features.