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Crystal Graph Neural Networks for Data Mining in Materials Science

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Abstract

Machine learning methods have been employed for materials prediction in various ways. It has recently been proposed that a crystalline material is represented by a multigraph called a crystal graph. Convolutional neural networks adapted to those graphs have successfully predicted bulk properties of materials with the use of equilibrium bond distances as spatial information. An investigation into graph neural networks for small molecules has recently shown that the no distance model performs almost as well as the distance model. This paper proposes crystal graph neural networks (CGNNs) that use no bond distances, and introduces a scale-invariant graph coordinator that makes up crystal graphs for the CGNN models to be trained on the dataset based on a theoretical materials database. The CGNN models predict the bulk properties such as formation energy, unit cell volume, band gap, and total magnetization for every testing material, and the average errors are less than the corresponding ones of the database. The predicted band gaps and total magnetizations are used for the metal-insulator and nonmagnet-magnet binary classifications, which result in success. This paper presents discussions about high-throughput screening of candidate materials with the use of the predicted formation energies, and also about the future progress of materials data mining on the basis of the CGNN architectures.

Full text link

GitHub repo: Tony-Y/cgnn