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Geometric learning for sampling atomic conformations

A material's atomic conformation dictates the resulting electronic and mechanical properties; therefore, determining the experimentally realizable conformation is a key task in molecular modeling. Ab initio approaches allow one to compute the relaxed conformation with high accuracy, albeit at high computational cost. Alternatively, high-throughput sampling methods allow one to quickly explore large areas of chemical space, but at reduced accuracy. Traditional Monte Carlo approaches to sampling atomic conformations rely on predefined structural perturbations of a structure's 3D point cloud, such as rotations around specific bonds or translations of specific atoms. However, in material systems under periodic boundary conditions, ideal sampling perturbations are not well defined as most material systems do not have covalent bonds around which to rotate and atom translations lead to cascading atomic motions across the entire material. Therefore, we redefine the problem to sample graphs, rather than 3D point clouds. We designed a graph neural network (GNN) to sample atomic conformations learned from a training set of relevant structures in lieu of predefined perturbations. This talk will discuss the definition of material graphs and sampling of new material graphs via GNN.