Modeling crystal defects using defect-informed neural networks

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1. Introduction

Machine learning has revolutionized the study of crystalline materials for enabling rapid predictions and discovery. However, most AI-for-Materials research to date has focused on ideal crystals, whereas real-world materials inevitably contain defects that play a critical role in modern functional technologies. The defects break geometric symmetry and increase interaction complexity, posing particular challenges for traditional ML models. Addressing these challenges requires models that are able to capture sparse defect-driven effects in crystals while maintaining adaptability and precision. Here, we introduce Defect-Informed Equivariant Graph Neural Network (DefiNet), a model specifically designed to accurately capture defect-related interactions and geometric configurations in point-defect structures. Trained on 14,866 defect structures, DefiNet achieves highly accurate structural predictions in a single step, avoiding the time-consuming iterative processes in modern ML relaxation models and possible error accumulation from iteration. We further validates DefiNet accuracy by using density functional theory (DFT) relaxation on DefiNet-predicted structures. For most defect structures, regardless of defect complexity or system size, only 3 ionic steps are required to reach the DFT-level ground state. Finally, comparisons with scanning transmission electron microscopy (STEM) images confirm DefiNet scalability and extrapolation beyond point defects, positioning it as a groundbreaking tool for defect-focused materials research.

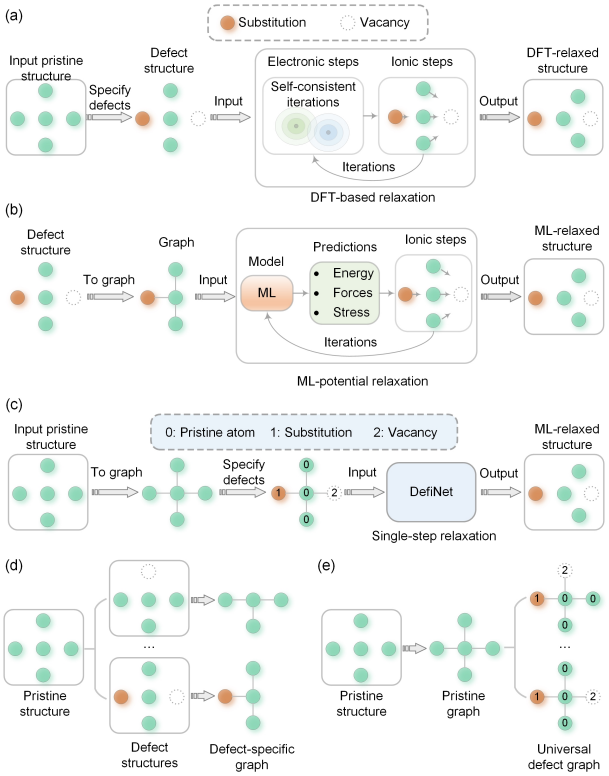

Fig. 1: Overview of crystal defect structure relaxation methods. (a) Relaxation using DFT with multi-step iterations. (b) Relaxation using ML potentials with multi-step iterations. (c) Relaxation using our DefiNet with a single step. (d) The traditional specific graph representation for defect structures. (e) Our proposed universal defect graph representation.

1.1 Figures and tables

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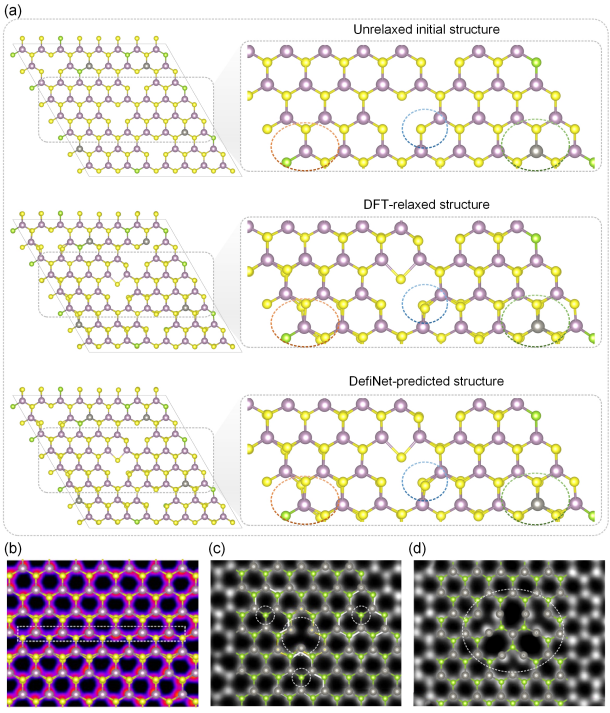

Fig. 2: Visualization of DefiNet-predicted defect structures and comparisons with STEM images. (a) Example of an MoS_2 crystal structure containing both substitutional and vacancy defects, alongside the corresponding DFT-relaxed and DefiNet-predicted structures. (b) STEM image of MoS_2 featuring a line defect, overlaid with the DefiNet-relaxed structure. Copyright 2016 American Chemical Society. (c) STEM image of WSe_2 with mixed SV_{Se} and DV_{Se} defects, overlaid with the DefiNet-relaxed structure. (d) STEM image of WSe_2 with a three-fold symmetrical trefoil defect, overlaid with the DefiNet-relaxed structure. Defect sites are highlighted with white dotted lines for clarity.