A Machine-Learning Approach to Boron Oxide Structures

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We present a novel simulation approach for boron oxide systems, focusing on the structural role of the boroxol ring. To address the complex nature of vitreous boron oxide (v-B_2O_3), we developed an efficient machine learning interatomic potential (MLIP) that was trained using density functional theory (DFT) across a range of densities, from random to crystalline phases. Our comprehensive analyses include the equation of state, structure factor, stabilization energy of the boroxol ring, and the ring-breaking process. A key finding is the significance of van der Waals (vdW) forces in determining crystal density and how the stability of the boroxol ring and its transition mechanisms shift with changes in density. This work provides deeper insights into the structural dynamics of boron oxide and demonstrates the potential of MLIPs for modeling complex atomic systems beyond traditional methods. Our study notably advances the understanding and exploration of boron oxide and similar materials in theoretical and applied materials science.

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