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Understanding the Structure and Mechanical Properties of ZIF Glasses by a Machine Learning Force Field

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The glassy state of metal-organic frameworks (MOFs) offers unique features, such as combining nano-porosity with lack of grain boundaries. Zeolitic imidazolate frameworks (ZIFs) are an important subset of MOFs that can form glasses through melt-quenching, but their structure-property relations have not yet been fully understood. To overcome this challenge, we here develop a deep learning force field (DLFF) for molecular dynamics (MD) simulations, which is able to reproduce both the structure and mechanical properties of ZIF glass with an accuracy comparable to *ab initio* MD, yet at a much lower computational cost. With this force field, we then reveal that the structural changes of the typical ZIF-4 glass under different temperatures and pressures mainly originate from the reorientation of imidazole rings. We also show that this DLFF is transferable to functionalized ZIF glasses outside the training sets and we use it to correlate local structural fingerprints with the mechanical properties. This work can thus guide the future design of MOF glasses with improved performances.