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Structural descriptors for zeolitic imidazolate framework glasses

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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, some of which can be vitrified to glass through melt-quenching, but their structure-property relations have not yet been fully understood. Based on a developed deep learning force field for molecular dynamics simulations, which is able to reproduce both the structure and mechanical properties of ZIF glasses, we study the structural origins of phase transitions and composition dependence of mechanical properties. Specifically, we discuss the role of various structural descriptors, such as ring orientation index and local entropy and volume of metal ions, in capturing these variations. The development of suitable structural descriptors is crucial for the future design of MOF glasses with improved performances.