Structural phase transitions in monolayer TMDs with a neural-network interatomic potential

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Among the wide family of layered materials, transition metal dichalcogenides (TMDs) constitute a broad class of systems exhibiting diverse properties depending on chemical composition, temperature, pressure, and dimensionality. In the single-layer limit, some TMDs, such as tungsten ditelluride (WTe_2) and molybdenum ditelluride ($MoTe_2$), exhibit distinct polymorphs. These materials showcase two dynamically stable phases characterized by a small energy difference, both of which can be experimentally observed.
Understanding the atomistic mechanisms governing the transitions between these competing phases requires an accurate yet computationally efficient description of the potential-energy surface. To this end, we employ neural-network interatomic potentials trained on density-functional-theory data through an active-learning campaigns carried out with AiiDA-TrainsPot. This workflow, which we recently developed, provides a computationally efficient and largely automated approach for training machine-learning potentials via active learning, while also delivering quantitative error estimates.
Using this potential, we characterized the structural phase transitions in $MoTe_2$ and WTe_2 polymorphs, which are separated by a high energy barrier. Our investigation elucidates the roles of defects, interfaces, and temperature in facilitating transitions from metastable to stable phases.
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