Rb melting curve and phase transitions at high pressure with Machine Learning

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Rb exhibits complex non-monotonous pressure dependence of the melting curve associated with phase transitions in the solid. Classical interaction potentials (e.g. EAM) have not succeeded to reproduce this experimentally observed phenomenon and extensive ab-initio studies of phase transitions are computationally expensive. In an attempt to circumvent the restricting nature of the physics-based assumptions of the classical potentials we utilize the more flexible Machine Learning schemes to generate the atomistic potential. In particular, we chose to employ Behler-scheme for neural-networks that are fed with a descriptor of radial and angular symmetry functions. Ab-initio molecular-dynamics simulations of 5-10 picoseconds at several pressures in the liquid and solid states constitute the training and test data. To predict the phase equilibrium temperatures we use the bi-phase method and construct supercells which are half solid and half liquid. These ML-MD simulations reach equilibrium after few tens of picoseconds, from which the melting curve for a given ML-potential can be constructed. Employing this approach we are able to reproduce salient properties of the Rb melting curve including the strong temperature dependence at low pressures and the maximum in the melting curve.