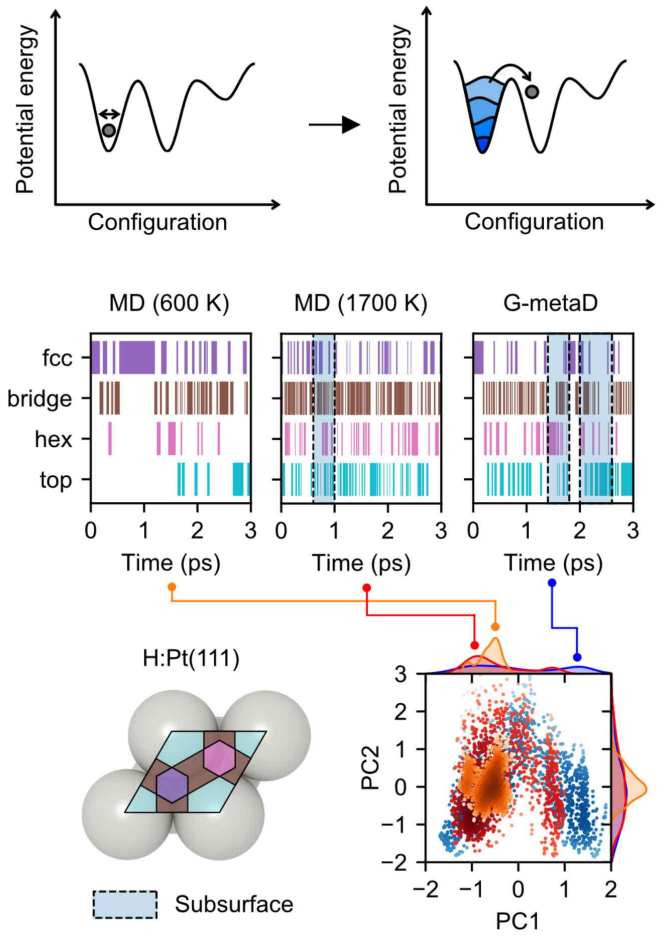
Metadynamics sampling for machine learning potentials



The machine learning potentials (MLPs) are garnering large attention, providing the accuracy of *ab initio* calculations at much lower costs. MLPs guarantee their reliability within the training domain. However, it requires expertise and enormous time to collect all necessary configurations by hand-picking. We suggest a sampling method via metadynamics accumulating on the local atomic environment space, which is called G-metaD. G-metaD is applied to H:Pt(111), GeTe, and Si systems. This work was accepted at npj Computational Materials.