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SNAP: Automated Generation of High-Accuracy Interatomic Potentials using Quantum Data[1] AIDAN THOMPSON, MITCHELL WOOD, Sandia Natl Labs, SIMON PHILLPOT, U. of Florida — Molecular dynamics simulation is a powerful computational method for bridging between macroscopic continuum models and quantum models treating a few hundred atoms, but it is limited by the accuracy of the interatomic potential. Sound physical and chemical understanding have led to good potentials for certain systems, but it is difficult to extend them to new materials and properties. The solution is obvious but challenging: develop more complex potentials that reproduce large quantum datasets. The growing availability of large data sets has made it possible to use automated machine-learning approaches for interatomic potential development. In the SNAP approach, the interatomic potential depends on a very general set of atomic neighborhood descriptors, based on the bispectrum components of the density projected onto the surface of the unit 3-sphere. Previously, this approach was demonstrated for tantalum, reproducing the screw dislocation Peierls barrier. In this talk, it will be shown that the SNAP method is capable of reproducing a wide range of energy landscapes relevant to diverse material science applications: i) point defects in indium phosphide, ii) stability of tungsten surfaces at high temperatures, and iii) formation of intrinsic defects in uranium.

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