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Title: Routines for basic tests of atomistic potentials with universal interface

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We present a set of Python routines to perform basic tests of classical atomistic potentials and their example applications. These routines are implemented using universal Atomistic Simulation Environment (ASE) and LAMMPS molecular dynamics code. ASE is utilized to create atomic configurations, to write input scripts for LAMMPS, and to read results from output files.

Evaluated properties are formation energies and volumes of simple point defects (vacancies, substitutions, and interstitials), formation energies of basic surfaces, heats of formation of simple binary compounds, and elastic constants. The flexibility of LAMMPS allows easy switching between varying semi-empirical potentials, while the universality of ASE allows to compare results with a number of ab-initio codes.