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Ab-initio Calculations for MEAM Potential of Al, Si, Mg, H, O and Cu Alloys BOHUMIR JELINEK, Mississippi State University, SEONG-GON KIM, Mississippi State University, MARK HORSTEMEYER, Mississippi State University, MICHAEL I. BASKES, Sandia National Laboratory — The ab-initio calculations based on the density functional theory (DFT) were performed for the Si, Al, Mg, H, O, Cu crystals and their pair combinations in reference structures, such as NaCl structure. The lattice constant (volume), bulk modulus and shear moduli for each pair were determined from the total energy calculations. These material parameters were then used to determine the Modified Embedded Atom Method (MEAM) potentials for these elements and their alloys. MEAM simulations that model the mechanical properties of these alloy materials will be presented to demonstrate the validity and transferability of the new MEAM potentials.

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