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Quantum-Based Atomistic Simulation of Transition Metals[1]

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First-principles generalized pseudopotential theory (GPT) provides a fundamental basis for *transferable* multi-ion interatomic potentials in transition metals and alloys within density-functional quantum mechanics. In central bcc transition metals, where multi-ion angular forces are important to structural properties, simplified *model* GPT or MGPT potentials have been developed based on canonical d bands to allow analytic forms and large-scale atomistic simulations. Robust, advanced-generation MGPT potentials have now been obtained for Ta and Mo and successfully applied to a wide range of structural, thermodynamic, defect and mechanical properties at both ambient and extreme conditions of pressure and temperature, including multiphase equation of state, melting and rapid resolidification, thermoelasticity and the detailed atomistic simulation of point defects, dislocations and grain boundaries needed for the multiscale modeling of plasticity and strength. Recent algorithm improvements have also allowed the implementation of a more general matrix representation of MGPT beyond canonical bands for increased accuracy and extension to f-electron actinide metals plus an order of magnitude increase in computational speed. An important further advance still in progress is the development of temperature-dependent MGPT potentials that subsume electron-thermal as well as ion-thermal contributions to high-temperature properties.

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