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Material Discovery and Design with Dynamic Charge Reactive Potentials

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Atomic scale computational simulations of multi-phase systems is increasingly important as our ability to simulate nanometer-sized systems becomes routine. The recently developed charge optimized many body potential (COMB) potentials have significantly enhanced our ability to carry out atomic-scale simulations of heterogeneous material systems. The formalism of this potential combines variable charge electrostatic interactions with a classical analytical bond-order potential. It therefore has the capacity to adaptively model metallic, covalent, ionic, and van der Waals bonding within the same simulation cell and dynamically determine the charges on individual atoms according to the local environment. The utility of the COMB potentials is illustrated for materials design and discovery by exploring the structure, stability, mechanical properties, and thermal properties of intermetallic systems and oxide-metal interfaces. They are also used to address key questions associated with corrosion, thin film growth, and heterogeneous catalysis.