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Next Generation Classical Potentials for Modeling Many-Body Interactions in Materials

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Reactive force fields, which are also called potentials, are used in atomic-scale simulations to predict interatomic forces and energies. The next generation of these force fields allow for the prediction of sophisticated chemical reactions at scales larger than can be achieved with first-principles quantum-based methods. This presentation will present several examples of charge optimized many-body (COMB) potentials being used in atomic-scale molecular dynamics and adaptive Monte Carlo simulations to model surface and heterogeneous interfacial chemistry.