Charge Optimized Many-Body (COMB) Potentials for Interfacial Studies

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Graphene has attracted tremendous attention owing to its interesting properties and unique structure. A key intermediate product in the chemical production of graphene is graphene oxide sheets, which are often heavily oxygenated with hydroxyl or epoxide functional groups on the surface and carbonyl or carboxyl groups at the edges. The energetics associated with the interaction of graphene sheets with various levels of oxidation with metal and oxide interfaces is examined in molecular dynamics simulations using charge optimized many-body (COMB) potentials, which enable the investigation of heterogeneous interfacial structures within a single unit cell. The properties of the COMB potentials and their applications to other heterogeneous interfacial systems will also be reviewed.