The Art and Science of Many-Body Reactive Potentials

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When many-body potentials for describing chemical reactions involving more than a few atoms were introduced in the 1980's, they were largely viewed with suspicion by much of the modeling community. More than a few papers from that era, for example, included sentences like "quantum mechanics is needed to model reactions..." and promoted constructs such as QM-MM as the only way to incorporate chemistry into condensed-phase simulations. What the authors of many of these papers failed to realize is that quantum concepts are introduced into the functional form of these potential energy expressions via quantities such as environment-dependent bond orders and embedding functions. As the utility of these early many-body reactive potentials was recognized by a broader modeling community their use expanded, while at the same time more sophisticated (and accurate) forms such as the ReaxFF and COMB potentials were introduced.

This talk will focus on why many-body potentials such as the reactive empirical bond-order expressions work as well as they do, in particular the quantum origins and parameter fitting strategies, and where improvements are still needed. Emerging strategies for extending capabilities and applications for many-body reactive potentials will also be discussed.