

Abstract Submitted
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Developing a Reactive Potential for Hydrocarbons Under Extreme Deformation¹ THOMAS O'CONNOR, Johns Hopkins University, LARS PASTEWKA, Fraunhofer Institute for Mechanics of Materials IWM, JAN ANDZELM, Army Research Laboratory, MARK ROBBINS, Johns Hopkins University — In traditional molecular dynamics, interaction potentials define and maintain a fixed topology of chemical bonds. The development of reactive cluster potentials, such as the AIREBO and the REAXFF, have allowed modelers to explore dynamic bonding processes at the expense of more complex many-particle interactions. The complexity of these many-particle interactions makes parameterization of such models difficult; consequentially, current cluster potentials quickly lose fidelity outside a limited range of ambient pressures and temperatures, corresponding to near equilibrium states of the bonds described. In order to accurately describe the dynamics of extreme loading and failure, existing reactive cluster potentials must be modified to improve the description of highly strained bond configurations. Here we present a modified AIREBO potential for hydrocarbons with accuracy extended to highly strained intra (and inter) molecular configurations. Implementing recently developed techniques of bond-screening and a reparameterization of van der Waal's interactions based on second-order Moller-Plesset perturbation theory, we explore the equilibrium states of condensed phase hydrocarbons under high pressure and yield under extreme loads.

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