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Analysis of Chemistry in Reactive Molecular Dynamics Simulations EDWARD KOBER, Los Alamos National Laboratory — The application of reactive molecular dynamics simulations to the reactions of energetic materials, especially for understanding ignition and deflagration processes in condensed phases, is now relatively common. However, the analyses of the reaction processes are often rather limited, restricted to following the appearance or disappearance of specific molecules. A more complete method of analysis is presented here. This is based on classifying each atom in the simulation by its coordination environment. This generates a countable matrix of geometry changes that can be formulated into a reduced chemistry model using Non-negative Matrix Factorization. This captures the general reaction characteristics (e.g. reduction of nitrogen, oxidation of carbon) in a series of correlated chemical waves. By analyzing simulations as a function of initial temperature and density, the Arrhenius reaction rates and thermodynamics properties can be extracted. Applications to HMX from ambient to detonation conditions using ReaxFF will be discussed.

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