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ReaxFF Predictions on Detonation Properties and Reaction Kinetics across the Energetic Materials[1] MD MAHBUBUL ISLAM, BRENDEN HAMILTON, MICHAEL SAKANO, PILSUN YOO, PEILIN LIAO, ALEJANDRO STRACHAN, Purdue University — Developing predictive capabilities to determine detonation and kinetics properties, as well as chemical decomposition mechanism is crucial for designing new energetic materials (EM). We use ReaxFF molecular dynamics simulations with Hugoniostat technique to predict detonation velocities, Chapman-Jouguet pressures, and NVT cook-offs to calculate activation barriers in a range of EMs such as NM, TNT, TATB, RDX, HMX, PETN, and CL-20. We employ four ReaxFF parametrizations to assess the uncertainties associated with the predictions stemmed from the choice of force fields. Across the materials and force fields, our predicted detonation velocities are found to be within 7-18% of the experiments and detonation products capture the trend in the experimental data. In order to further improve the accuracy of the predictions, we are currently working to incorporate atom and bond type dependent linear correction terms to the ReaxFF. The coefficients of the linear corrections are being fitted against the discrepancies in forces and energies between ReaxFF and quantum chemistry calculations. Such development will be an important step towards more accurate predictions of the properties of the EMs.

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