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Machine Learning Reactive Force Fields for an Atomistically-Resolved View into Shockwave-Driven Carbon Condensation

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In this work, we discuss development and application of the Chebyshev Interaction Model for Efficient Simulations (ChIMES) to the problem of carbon condensation. Formation of soot particles resulting from strong shockwave propagation in carbon-rich energetic materials can have significant implications on material performance and sensitivity. However, the time and length scales associated with condensate growth (i.e. up to hundreds of ns and 10's of nm, respectively) make direct investigation highly challenging. From an experimental standpoint, these scales preclude formation tracking, leading to what appears to be instantaneous condensate growth, while for highly predictive quantum-based simulation methods, these scales are prohibitively large. Reactive force field-based approaches, capable of multi-million atom simulations, offer a viable alternative means of studying carbon condensation. To this effect, we discuss development of the Chebyshev Interaction Model for Efficient Simulation (ChIMES), a generalized many-body reactive force field machine-learned to Kohn-Sham Density Functional Theory (DFT) molecular dynamics trajectories. ChIMES models are linear-scaling with respect to system size and are thus highly suitable for large-scale problems requiring atomistic resolution. Strategies for achieving "quantum-accurate" descriptions of chemistry in complicated molecular systems are discussed and broad insights stemming from application to carbon condensation in liquid carbon monoxide under extreme conditions are presented. Our results indicate possible mechanisms, timescales, and chemistry for the ensuing condensate products. In collaboration with: L.E. Fried, N. Goldman, S. Bastea and M.R. Armstrong This work is performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. LLNL-ABS-768127