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Reactive Force Field for Liquid Hydrazoic Acid with Applications to Detonation Chemistry[1] DAVID FURMAN, Hebrew University of Jerusalem and NRCN, israel, FAINA DUBNIKOVA, Hebrew University of Jerusalem, Israel, ADRI VAN DUIN, Penn. State University, Pennsylvania, USA, YEHUDA ZEIRI, Ben Gurion University, Israel and NRCN, Israel, RONNIE KOSLOFF, Hebrew University of Jerusalem, Israel — The development of a reactive force field (ReaxFF formalism) for Hydrazoic acid (HN3), a highly sensitive liquid energetic material, is reported. The force field accurately reproduces results of density functional theory (DFT) calculations. The quality and performance of the force field are examined by detailed comparison with DFT calculations related to uni, bi and trimolecular thermal decomposition routes. Reactive molecular dynamics (RMD) simulations are performed to reveal the initial chemical events governing the detonation chemistry of liquid HN3. The outcome of these simulations compares very well with recent results of tight-binding DFT molecular dynamics and thermodynamic calculations. Based on our RMD simulations, predictions were made for the activation energies and volumes in a broad range of temperatures and initial material compressions.

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