Abstract Submitted
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Theoretical Characterizaiton of Visual Signatures (Muzzle Flash)[1] D.O. KASHINSKI, A.N. SCALES, D.L. VANDERLEY, G.M. CHASE, O.E. DI NALLO, United States Military Academy, E.F.C. BYRD, Army Research Laboratory — We are investigating the accuracy of theoretical models used to predict the visible, ultraviolet and infrared spectra of product materials ejected from the muzzle of currently fielded systems. Recent advances in solid propellants has made the management of muzzle signature (flash) a principle issue in weapons development across the calibers. *A priori* prediction of the electromagnetic spectra of formulations will allow researchers to tailor blends that yield desired signatures and determine spectrographic detection ranges. We are currently employing quantum chemistry methods at various levels of sophistication to optimize molecular geometries, compute vibrational frequencies, and determine the optical spectra of specific gas-phase molecules and radicals of interest. Electronic excitations are being computed using Time Dependent Density Functional Theory (TD-DFT). A comparison of computational results to experimental values found in the literature is used to assess the affect of basis set and functional choice on calculation accuracy. The current status of this work will be presented at the conference.

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