Abstract Submitted
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Theoretical Characterizaiton of Visual Signatures[1] D.O. KASHINSKI[2], G.M. CHASE, O.E. DI NALLO, A.N. SCALES, D.L. VANDERLEY, 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, as well as other properties, 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. Quantum chemistry methods at various levels of sophistication have been employed to optimize molecular geometries, compute unscaled vibrational frequencies, and determine the optical spectra of specific gas-phase species. Electronic excitations are being computed using Time Dependent Density Functional Theory (TD-DFT). A full statistical analysis and reliability assessment of computational results is currently underway. A comparison of theoretical results to experimental values found in the literature is used to assess any affects of functional choice and basis set on calculation accuracy. The status of this work will be presented at the conference.

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D.O. Kashinski
United States Military Academy

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