

Abstract Submitted  
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**Optical characterization of shock-induced chemistry in the explosive nitromethane using DFT and time-dependent DFT<sup>1</sup>** LENSON PELLOUCHOUD, EVAN REED, Stanford University — With continual improvements in ultrafast optical spectroscopy and new multi-scale methods for simulating chemistry for hundreds of picoseconds, the opportunity is beginning to exist to connect experiments with simulations on the same timescale. We compute the optical properties of the liquid phase energetic material nitromethane ( $\text{CH}_3\text{NO}_2$ ) for the first 100 picoseconds behind the front of a simulated shock at 6.5km/s, close to the experimentally observed detonation shock speed. We utilize molecular dynamics trajectories computed using the multi-scale shock technique (MSST) for time-resolved optical spectrum calculations based on both linear response time-dependent DFT (TDDFT) and the Kubo-Greenwood (KG) formula within Kohn-Sham DFT. We find that TDDFT predicts optical conductivities 25-35% lower than KG-based values and provides better agreement with the experimentally measured index of refraction of unreacted nitromethane. We investigate the influence of electronic temperature on the KG spectra and find no significant effect at optical wavelengths. With all methods, the spectra evolve non-monotonically in time as shock-induced chemistry takes place. We attribute the time-resolved absorption at optical wavelengths to time-dependent populations of molecular decomposition products, including NO, CNO, CNOH,  $\text{H}_2\text{O}$ , and larger molecules.

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