269. Title: A general framework for numerical simulation of improvised explosive device (IED)-detection scenarios using density functional theory (DFT) and terahertz (THz) spectra

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Abstract: We have developed a general framework for numerical simulation of various types of scenarios that can occur for the detection of improvised explosive devices (IEDs) through the use of excitation using incident electromagnetic waves. A central component model of this framework is an S-matrix representation of a multilayered composite material system. Each layer of the system is characterized by an average thickness and an effective electric permittivity function. The outputs of this component are the reflectivity and the transmissivity as functions of frequency and angle of the incident electromagnetic wave. The input of the component is a parameterized analytic-function representation of the electric permittivity as a function of frequency, which is provided by another component model of the framework. The permittivity function is constructed by fitting response spectra calculated using density functional theory (DFT) and parameter adjustment according to any additional information that may be available, e.g., experimentally measured spectra or theory-based assumptions concerning spectral features. A prototype simulation is described that considers response characteristics for THz excitation of the high explosive ß-HMX. This prototype simulation includes a description of a procedure for calculating response spectra using DFT as input to the Smatrix model. For this purpose, the DFT software NRLMOL was adopted.