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Title

THz Dielectric Properties of High Explosives Calculated by Density Functional Theory for the Design of Detectors

Source

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Abstract

The current need for better detection of explosive devices has imposed a new necessity for determining the dielectric response properties of energetic materials with respect to electromagnetic wave excitation. Among the range of different frequencies for electromagnetic excitation, the THz frequency range is of particular interest because of its nondestructive nature and ability to penetrate materials that are characteristic of clothing. Typically, the dielectric response properties for electromagnetic wave excitation at THz frequencies, as well as at other frequencies, are determined by means of experimental measurements. The present study, however, emphasizes that density functional theory (DFT), and associated software technology, is sufficiently mature for the determination of dielectric response functions, and actually provides complementary information to that obtained from experiment. In particular, these dielectric response functions provide quantitative initial estimates of spectral response features that can be adjusted with respect to additional information such as laboratory measurements and other types of theory-based calculations, as well as providing for the molecular level interpretation of response structure. This point is demonstrated in the present study by calculations of ground-state resonance structure associated with the high explosives RDX, TNT1, and TNT2 using DFT, which is for the construction of parameterized dielectric response functions for excitation by electromagnetic waves at frequencies within the THz range. The DFT software NRLMOL was used for the calculations of ground-state resonance structure presented here.