

155

Accession number:20123515377139

Title:Dielectric response of high explosives at THz frequencies calculated using density functional theory

Authors:Huang, L. (1); Shabaev, A. (2); Lambrakos, S.G. (1); Bernstein, N. (1); Jacobs, V. (1); Finkenstadt, D. (3); Massa, L. (4)

Author affiliation:(1) Naval Research Laboratory, Washington, DC 20375, United States; (2) George Mason University, Fairfax, VA 22030, United States; (3) Physics Department, U.S. Naval Academy, Annapolis, MD 21402, United States; (4) Hunter College, CUNY, New York, NY 10065, United States

Corresponding author:Lambrakos, S.G.(lambrakos@anvil.nrl.navy.mil)

Source title:Journal of Materials Engineering and Performance

Abbreviated source title:J Mater Eng Perform

Volume:21

Issue:7

Issue date:July 2012

Publication year:2012

Pages:1120-1132

Language:English

ISSN:10599495

CODEN:JMEPEG

Document type:Journal article (JA)

Publisher:Springer New York, 233 Spring Street, New York, NY 10013-1578, United States

Abstract:We present in this study calculations of the ground-state resonance structures associated with the high explosives  $\beta$ -HMX, PETN, RDX, TNT1, and TNT2 using density functional theory (DFT). Our objective is the construction of parameterized dielectric-response functions for excitation by electromagnetic waves at compatible frequencies. These dielectric-response functions provide the basis for analyses pertaining to the dielectric properties of explosives. In particular, these dielectric-response functions provide quantitative initial estimates of spectral-response features for subsequent adjustment with knowledge of additional information, such as laboratory measurements and other types of theory-based calculations. With respect to qualitative analyses, these spectra provide for the molecular-level interpretation of response structure. The DFT software GAUSSIAN was used for the calculations of the ground-state resonance structures presented here. © ASM International.

Number of references:18

Main heading:Density functional theory

Controlled terms:Chemical analysis - Dielectric properties - Electric excitation - Explosives - Ground state

Uncontrolled terms:Density functional theories (DFT) - Dielectric response - Gaussians - High explosives - Initial estimate - Laboratory measurements - Material selection - Modeling process - Molecular levels - Parameterized - Qualitative analysis - Resonance structure - THz frequencies

Classification code:933.3 Electronic Structure of Solids - 933 Solid State Physics - 932 High Energy Physics; Nuclear Physics; Plasma Physics - 804 Chemical Products Generally - 801 Chemistry - 701.1 Electricity: Basic Concepts and Phenomena - 701 Electricity and Magnetism

DOI:10.1007/s11665-011-0020-3

Database:Compendex

Compilation and indexing terms, Copyright 2012 Elsevier Inc.