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Comparative Study of Electronic and Optical Properties of Ammonium and Potassium Dinitramide Salts through Ab-Initio Calculations

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Abstract : The present study investigates the role of ammonium and potassium ion in the electronic, bonding and optical properties of dinitramide salts due to their stability and non-toxic nature. A detailed analysis of bonding between NH_4 and K with dinitramide, optical transitions from the valence band to the conduction band, absorption spectra, refractive indices, reflectivity, loss function are reported. These materials are well known as oxidizers in solid rocket propellants. In the present work, we use full potential linear augmented plane wave (FP-LAPW) method which is implemented in the Wien2k package within the framework of density functional theory. The standard DFT functional local density approximation (LDA) and generalized gradient approximation (GGA) always underestimate the band gap by 30-40% due to the lack of derivative discontinuities of the exchange-correlation potential with respect to an occupation number. In order to get reliable results, one must use hybrid functional (HSE-PBE), GW calculations and Tran-Blaha modified Becke-Johnson (TB-mBJ) potential. It is very well known that hybrid functionals GW calculations are very expensive, the later methods are computationally cheap. The new developed TB-mBJ functionals use information kinetic energy density along with the charge density employed in DFT. The TB-mBJ functionals cannot be used for total energy calculations but instead yield very much improved band gap. The obtained electronic band gap at gamma point for both the ammonium dinitramide and potassium dinitramide are found to be 2.78 eV and 3.014 eV with GGA functional, respectively. After the inclusion of TB-mBJ, the band gap improved by 4.162 eV for potassium dinitramide and 4.378 eV for ammonium dinitramide. The nature of the band gap is direct in ADN and indirect in KDN. The optical constants such as dielectric constant, absorption, and refractive indices, birefringence values are presented. Overall as there are no experimental studies we present the improved band gap with TB-mBJ functional following with optical properties.

Keywords : ammonium dinitramide, potassium dinitramide, DFT, propellants
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