Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Optical and Electronic Properties of Diisopropylammonium Bromide molecular ferroelectric crystal (DIPAB) AHMAD ALSAAD, Jordan university of Science and Technology, NABIL AL-AQTASH, RENAT SABIRIANOV, University of Nebraska at Omaha — Diisopropylammonium Bromide molecular ferroelectric crystal (DIPAB) could be considered as a potential alternative for perovskite ferroelectric materials. We report the results of *ab-initio* calculations of electronic band structure and density of states to underline and explain the optical properties of $P2_1$ ferroelectric phase of DIPAB. In particular, we present the results on complex dielectric function, absorption, reflectivity, energy-loss spectra, and complex refractive index as functions of the frequency of the incident electromagnetic wave. We found that the optical band gap of the polar ferroelectric phase of DIPAB is ≈ 5 eV consistent with the steepest rise in the absorption spectra. Furthermore, we found that the ferroelectric phase of DIPAB exhibits two fundamental oscillator bands at 5.91 and 6.4 eV, which correspond to the optical transitions from the valence band of bromine to the conduction band of nitrogen and carbon. Analysis of optical spectra in the 0–4.8 eV photon energy range reveals that this phase is characterized by high transparency, no absorption and a small reflectivity in this range. We found that the sharp maxima in the energy-loss occur at 14.35 and 15.82 eV in polar phase. The peak value of volume loss, 15.82 eV in polar phase, coincides with the zero values of the real part of the corresponding dielectric functions.

Ahmad Alsaad
Jordan university of Science and Technology

Date submitted: 14 Nov 2014 Electronic form version 1.4