

Abstract Submitted  
for the SHOCK11 Meeting of  
The American Physical Society

**Effect of impurities on optical properties of Pentaerythritol Tetranitrate (PETN)**<sup>1</sup> ROMAN TSYSHEVSKIY, Kazan State Technological University, MAIJA KUKLJA, University of Maryland College Park — Optical properties of an PETN molecule and a perfect crystal were studied to provide an interpretation to experimental data concerning to explosive decomposition of PETN caused by Nd:YAG laser irradiation (at 1064nm) (Aluker et al, J Phys Chem, 2011). We established that the HOMO-LUMO gap in a PETN molecule calculated using Gaussian09 program falls into the range of 5.7 to 6.8 eV, and the energy of the lowest singlet-triplet vertical transition requires 3.6-4.3 eV. The band gap of a perfect PETN calculated with VASP code is 4.2 eV. The obtained results show that the optical absorption of an ideal PETN requires the much higher energy than observed in experiment (1.17 eV). This discrepancy rules out the band transitions and suggests that defects induce a new low intensity optical absorption band in PETN. We simulate electronic excitations of possible impurities and compare them to optical properties of both ideal PETN crystals and real samples. Based on the obtained data, we propose a model for the laser initiation of PETN.

<sup>1</sup>This work is supported in part by ONR grantN00014-09-1-0225 and NSF.

Roman Tsyshevskiy  
Kazan State Technological University

Date submitted: 13 Apr 2011

Electronic form version 1.4