Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

PETN, RDX, HMX, TATB: band gap dependence on pressure under hydrostatic compression from DFT with GW and vdW corrections
ANDREI MUKHANOV, ALEXEI YANILKIN, Federal State Unitary Enterprise "All-Russia Research Institute of Automatics" — In the middle of 1990s Gilman (Gilman J. J. 1995 Phil. Mag. B, 71:6, 1057) proposed the idea that explosives transit from insulator to conductor state with following adiabatic expansion of free electrons in shockwave. One of the reasons of such a behavior of electrons is narrowing or disappearing of the fundamental band gap in explosive single crystal. It is well known that similar behavior can be simulated by DFT. But there is a severe problem of lowering the value of gap by DFT. So for quantitative prediction of narrowing of gap under pressure it is necessary to use more complicated methods like GW. From first principle calculations we determined elastic moduli for ideal crystals of PETN, RDX, HMX, and TATB. Accounting for those moduli we simulated the 0 K isotherms for hydrostatic compression of single crystal. Due to the essential role of van der Waals interaction in such materials the vdW corrections to DFT in Grimme's form was used. We obtained the dependencies for band gap on pressure under hydrostatic compression. Our preliminary results on GW calculations show that for TATB at initial uncompressed volume we have the value of gap twice a bigger in GW than in DFT.

Andrei Mukhanov
Federal State Unitary Enterprise "All-Russia Research Institute of Automatics"

Date submitted: 15 Nov 2013 Electronic form version 1.4