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Excitation energies of electrons in molecules & crystals of PETN, RDX, HMX, and TATB ANDREI MUKHANOV, VLADIMIR STEGAILOV, Federal State Unitary Enterprise "All-Russian Research Institute of Automatics" — The key role in the model of detonation based on metallization of explosive plays the fundamental band gap of molecular crystal. For determining it in shocked crystal we performed prerequisite calculations for ideal PETN, RDX, HMX and TATB at ambient conditions. Density of states for these explosives was obtained and fundamental gap was determined. Calculations were done within the framework of Density Functional Theory and its planewave and pseudopotential implementation in the ABINIT package [1]. Beside we determined excitation energies of electrons for isolated molecules of these explosives and compared it with fundamental gaps for crystals. [1] ABINIT : First-principles approach of materials and nanosystem properties. X. Gonze, B. Amadon, P.-M. Anglade, J.-M. Beuken, F. Bottin, P. Boulanger, F. Bruneval, D. Caliste, R. Caracas, M. Cote, T. Deutsch, L. Genovese, Ph. Ghosez, M. Giantomassi S. Goedecker, D.R. Hamann, P. Hermet, F. Jollet, G. Jomard, S. Leroux, M. Mancini, S. Mazevet, M.J.T. Oliveira, G. Onida, Y. Pouillon, T. Rangel, G.-M. Rignanese, D. Sangalli, R. Shaltaf, M. Torrent, M.J. Verstraete, G. Zerah, J.W. Zwanziger Computer Phys. Comm. 180, 2582-2615 (2009).

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