USING CARBONYL PHOTOINITIATORS FOR ACHIEVING TUNABLE OPTICAL SENSITIVITY OF PETN

ANTON ZVEREV[1, 2, 3], *ANATOLY MITROFANOV*[1, 2, 3], *ROMAN TSYSHEVSKY*[1], *MIKHAIL KOSTYANKO*[1], *SERGEY LUZGAREV*[1], *GUZEL GARIFZIANOVA*[5] *AND MAIJA KUKLJA*[4]

[1]*Kemerovo State University, Russia*
[2]*Yurga Institute of Technology, Russia*
[3]*National Research Tomsk Polytechnic University, Russia*
[4]*University of Maryland, USA*
[5]*Kazan National Research Technological University, Russia*
anthon.zverev@yandex.ru

Photo decomposition of wide gap dielectric PETN (Egap ~ 7 eV) doped with 9, 10-phenanthrenequinone (PQ) was triggered by irradiating samples with the laser beam with E ~2.33 eV. DFT modeling was employed to study optical properties of the pristine compounds and their mixture as well as for modeling decomposition mechanism on ground state and the lowest triplet potential energy surface. It was revealed that PQ molecule absorbs light in the range 1.9–2.4 eV. The excited PQ molecule abstracts hydrogen from the PETN which triggers subsequent barrierless cleavage of O-NO_2 bond. This reaction requires 9 kcal/mol, and proceeds with the heat release of 37.6 kcal/mol.

Keywords: *carbonyl photoinitiators, laser ignition, PETN.*