Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

Achieving tunable sensitivity in composite high-energy density materials SERGEY RASHKEEV, ROMAN TSYSHEVSKY, University of Maryland, MAIJA KUKLJA, National Science Foundation — Laser irradiation provides a unique opportunity for selective, predictive, and controlled initiation of energetic materials. We propose a consistent micro-scale mechanism of photoexcitation at the interface, formed by a molecular energetic material and a metal oxide. A specific PETN-MgO model composite is used to illustrate and explain seemingly puzzling experiments on selective laser initiation of energetic materials, which reported that the presence of metal oxide additives triggered the photoinitiation by an unusually low energy. We suggest that PETN photodecomposition is catalyzed by oxygen vacancies (F^0 centers) at the MgO surface. The proposed model suggests ways to tune sensitivity of energetic molecular materials to photoinitiation. Our quantum-chemical calculations suggest that the structural defects (e.g., oxygen vacancies) strongly interact with the molecular material (e.g., adsorbed energetic molecules) by inducing a charge transfer at the interface and hence play an imperative role in governing both energy absorption and energy release in the system. Our approach and conclusions provide a solid basis for novel design of energetic interfaces with desired properties and offers a new perspective in the field of explosive materials and devices.

Maija Kuklja
National Science Foundation

Date submitted: 29 Jan 2015 Electronic form version 1.4