Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

**Elucidation of high sensitivity of $\delta$-HMX: New insight from the first principle simulations** MAIJA KUKLJA, National Science Foundation, ONISE SHARIA, ROMAN TSYSHEVSKY, University of Maryland — Understanding of a tremendous difference in sensitivities of $\beta$ and $\delta$ phases of cyclotetramethylene-tetranitramine (HMX) has been long one of the stubborn challenges in the field of high energy density materials. Despite many experimental and theoretical efforts to explain the high sensitivity of the $\delta$ phase, convincing reasons behind the HMX behavior remained puzzling. We established that the presence of a polar surface in $\delta$-HMX has fundamental implications for stability and overall chemical behavior of the material. A comparative state-of-the-art quantum-chemical analysis of major decomposition mechanisms in polar $\delta$-HMX and nonpolar $\beta$-HMX discovered a dramatic difference in dominating dissociation reactions, activation barriers, and reaction rates. The polarization-induced charge transfer offered a logical explanation for different sensitivity of $\beta$-HMX and $\delta$-HMX polymorphs to detonation initiation. Our conclusions also removed long-standing contradictions and explained a large range of experimental data on thermal decomposition of HMX.

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Date submitted: 29 Jan 2015 Electronic form version 1.4