Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Molecular Mechanisms in the shock induced decomposition of FOX-7[1] ANKIT MISHRA, SUBODH C. TIWARI, CACS, USC, AIICHIRO NAKANO, PRIYA VASHISHTA, RAJIV KALIA, CACS, Department of Physics and Astronomy, Department of Chemical Engineering and Materials Science, CACS TEAM — Experimental and first principle computational studies on FOX 7 have either involved a very small system consisting of a few atoms or they did not take into account the decomposition mechanisms under extreme conditions of temperature and pressure. We have performed a large-scale reactive MD simulation using ReaxFF-lg force field to study the shock decomposition of FOX 7. The chemical composition of the principal decomposition products correlates well with experimental observations. Furthermore, we observed that the production of N_2 and H_2O was inter molecular in nature and was through different chemical pathways. Moreover, the production of CO and CO_2 was delayed due to production of large stable C,O atoms cluster. These critical insights into the initial processes involved in the shock induced decomposition of FOX-7 will greatly help in understanding the factors playing an important role in the insensitiveness of this high energy material.

[1]This research is supported by AFOSR award no. FA9550-16-1-0042.

Ankit Mishra
Univ of Southern California

Date submitted: 10 Nov 2016 Electronic form version 1.4