Abstract Submitted
for the SHOCK09 Meeting of
The American Physical Society

**Novel Catalytic Behavior of Water in High Explosive Decomposition** LAURENCE FRIED, CHRISTINE WU, LIN YANG, NIR GOLDMAN, SORIN BASTEA, Lawrence Livermore National Laboratory — Water under conditions of extremely high pressure and temperature is known to exhibit fascinating physical behaviors. Its remarkable structural and phase complexity strongly suggests that its chemical properties, which are largely unstudied, may be unusual as well. Detonations of high explosives containing oxygen and hydrogen provide unique systems for exploring the chemistry of "extreme water," because detonations form water at conditions similar to those of giant planetary interiors. Contrary to the current view of water as a stable final product, we show here that water plays an unexpected role in catalyzing complex explosive reactions. From first-principles atomistic simulations of the high explosive pentaerythritol tetranitrate (PETN), we discovered that $H_2O$ (source), H (reducer) and OH (oxidizer) act as a dynamic team that transports oxygen between reactive centers. Our finding suggests that $H_2O$ may catalyze reactions in other explosives and in planetary interiors. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Laurence Fried
Lawrence Livermore National Laboratory

Date submitted: 24 Feb 2009 Electronic form version 1.4