We study initiation and decomposition reactions in various energetic materials (EM) such as rocket propellants (hydrazine, methyl-hydrazine, and aluminum-powder based composites) and high explosives (pentaerythritol tetranitrate (PETN), octogen (HMX), hexogen (RDX), triaminotrinitrobenzene (TATB), and triacetone triperoxide (TATP)) using nonequilibrium molecular dynamics (MD) simulations with first principles-based reactive force field ReaxFF.

Such simulations are essential to elucidate atomistic mechanisms of condensed phase exothermic chemistry and detonation as well as their sensitivity to heat or impact stimuli. It can be applied for developing efficient rocket propellants, munitions, etc. with increased safety and survivability while retaining or improving performance as well as designing sensors and detectors with enhanced sensitivity to prevent terrorist attacks with improvised explosive devices (IED). In particular, development of solid composite propellants and prediction of their performance depending on composition and nanostructure requires understanding of detailed kinetics and combustion mechanism of nanoparticles as well as their melting and burning rates at the gas/surface interface.

The key concepts that enable ReaxFF to describe such processes with chemical reactions are: 1) the use of partial bond orders (a many body contribution based purely on atomic positions) to describe covalent interactions, 2) environment dependent atomic charges (updated at every step during the dynamics) to describe electrostatics, and 3) extensive validation by quantum mechanics calculations.

We investigate the influence of various factors on the decomposition of energetic materials and propellants including temperature, density/pressure, and heating/shock rates. Besides, we also perform simulations to identify early steps in initiation of chemical reactions, intermediates, and secondary products during combustion or detonation of energetic materials. We also studied effect of metals on propellant combustion such as catalyst-facilitated decomposition of hydrazine on Pt(100) surface or an increase of specific impulse (ISP) and energy release by embedding Al/Al2O3 nanoparticles into explosive matrix (RDX or PETN), as well as kinetics of carbon clustering during thermal decomposition of TATB and HMX.