A Computational Study of Dimethyl-Hydrazine Combustion

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The combustion of a specific rocket fuel, the unsymmetric Dimethyl-Hydrazine, $H_2NN(CH_3)_2$, commonly referred to as UDMH, is studied using computational techniques of *ab initio* molecular dynamics (AIMD) using VASP software.[1] The stoichiometric mixture of UDMH and nitrogen tetroxide, N_2O_4 in both the presence and absence of a platinum Nano catalyst is prepared at different values of temperature and density as the initial conditions for AIMD. A range of initial conditions is explored in an attempt to identify critical values of temperature and density; at low temperatures and density the reactants stay intact, while high temperature and densities demonstrate self-ignition of the reactants. As temperature is increased there becomes additional reaction pathways, which are indicative to higher activation energy. There are several possible products for this reaction, which include NO_2, NH_3, CO, CO_2, and steam (H_2O), shown in **Figure 1**. The aim of this work is to determine the environment for control of the dimethyl hydrazine self-ignition.

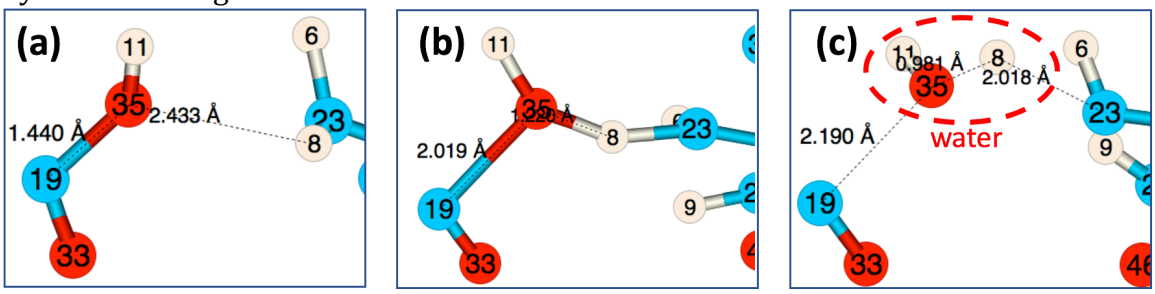

Figure 1. AIMD snapshots for typical reaction of hydrogen depriving from fuel to oxygen of oxidizer, resulting in water as a product. (a) reactants, (b) intermediates, (c) products. Images show small fragment of larger simulation cell.

1. Kresse, G.; Furthmuller, J., Efficient Iterative Schemes for Ab Initio Total-Energy Calculations Using a Plane-Wave Basis Set. *Phys. Rev. B* **1996,** *54* (16), 11169-11186.