

## Supplementary materials

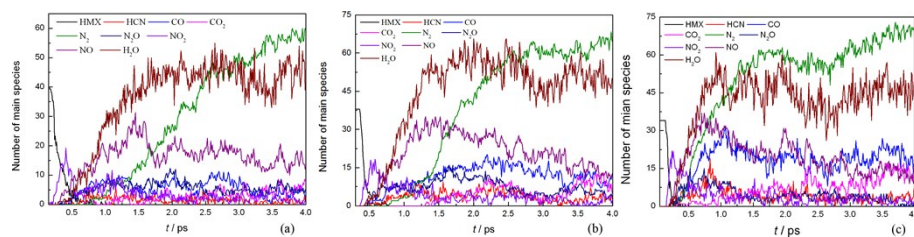


Fig. S1 Main species evolution involved in HMX decomposition: (a) perfect model, (b) model with two-molecule vacancy, (c) model with six-molecule vacancy

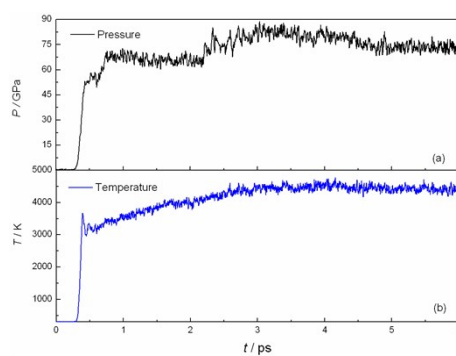


Fig. S2 Temperature and Pressure evolutions of HMX decomposition system

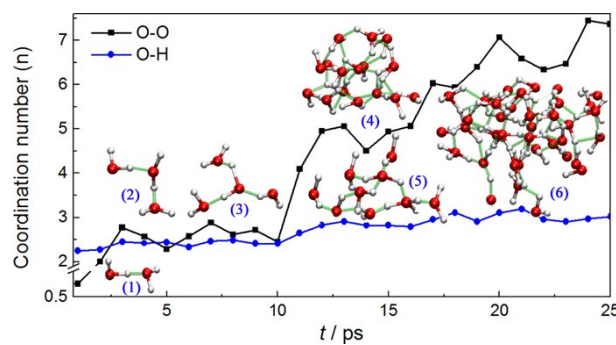


Fig. 3S Coordination number and corresponding typical structures of intermediate-water (green line represented the quasi hydrogen-bonds)