Nature of the Higher Self-heating Ability of Imperfect Energetic Crystals Relative to Perfect Ones

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Supporting Information (SI)

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S1. An experimental determination of peak temperatures of HMX decomposition at various heating rates.
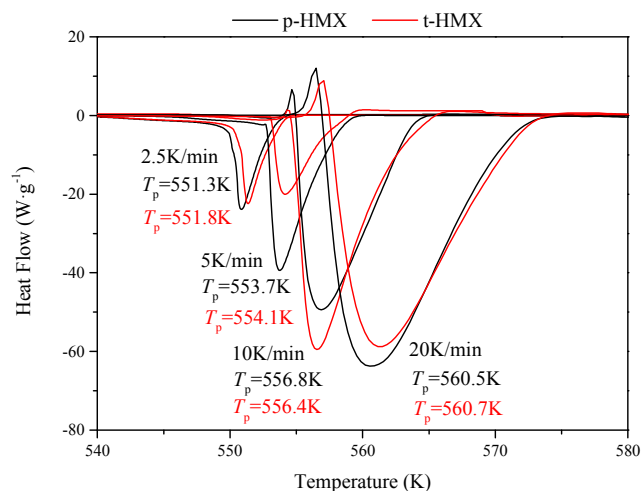

Figure s1. DSC tests of p-HMX and t-HMX samples at various heating rates.

The DSC measurements in a range of 23–400 °C were performed on a TA Instruments Discovery with perfect and twinned samples of ~1.5 mg and heating rates of 2.5-20 K/min. A nitrogen gas flow of 20 mL/min was maintained through the furnace during measurements. The DSC traces were analyzed using TROIS Analysis Software of TA Instruments.
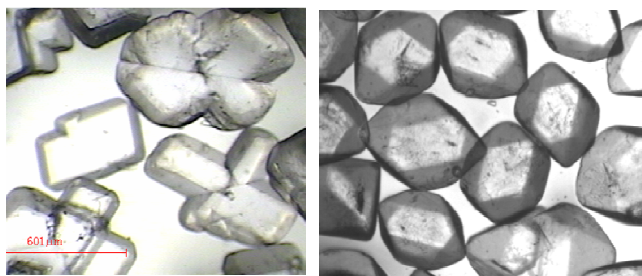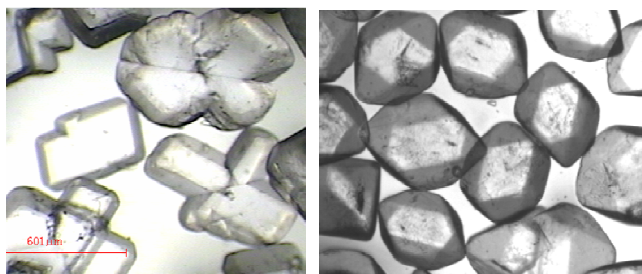
Figure s2. Optical imagines of the HMX crystals.

S2. Evolution of the main intermediates and products during thermal decay of HMX under constant temperature heating conditions.
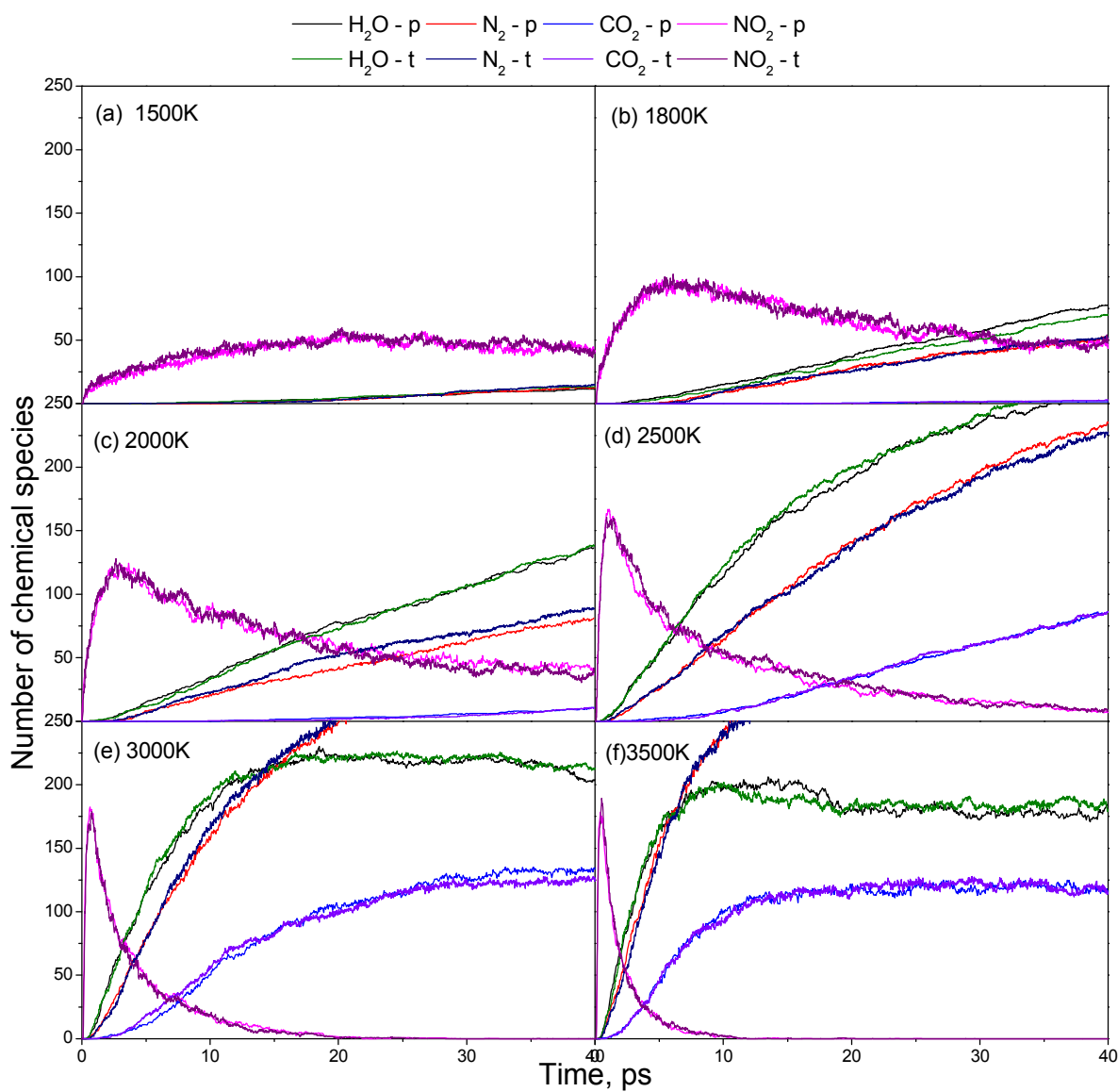

Figure s3. Evolution of the main intermediates and products.

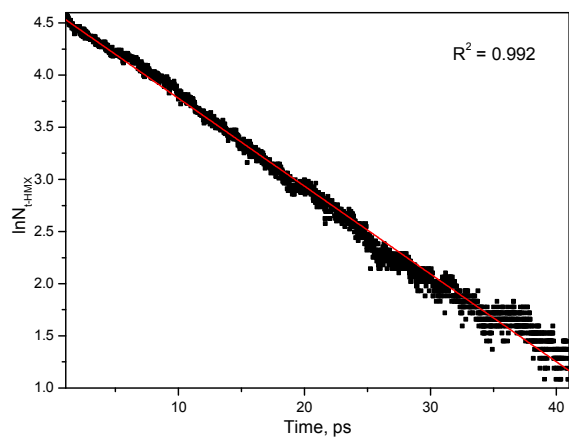## S3. Fitting for calculating kinetic constants.

$R^2 = 0.992$

Figure s4. Linear fitting of $lnN_{t\text{-}HMX}$ and time (t) of t-HMX decay at 1500 K.
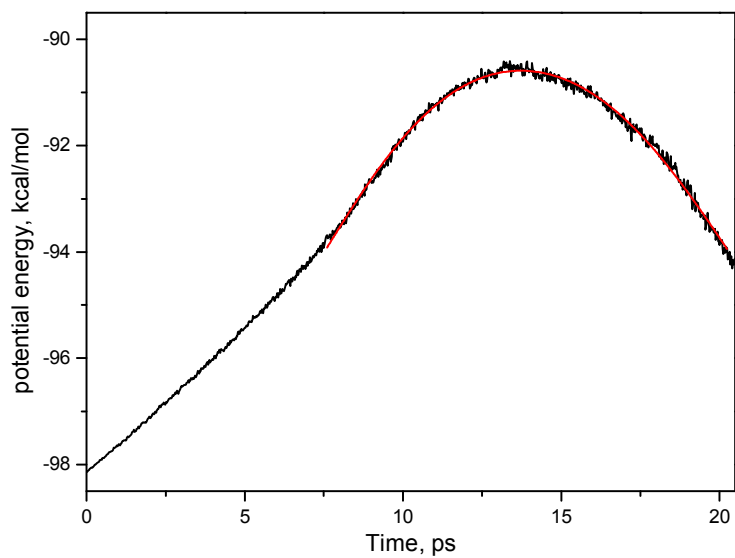

Figure s5. Single peak fitting to obtain the peak time for p-HMX at rate of 167 K/ps.

S4. Evolution of the main intermediates and products during thermal decay of HMX under programmed heating conditions.
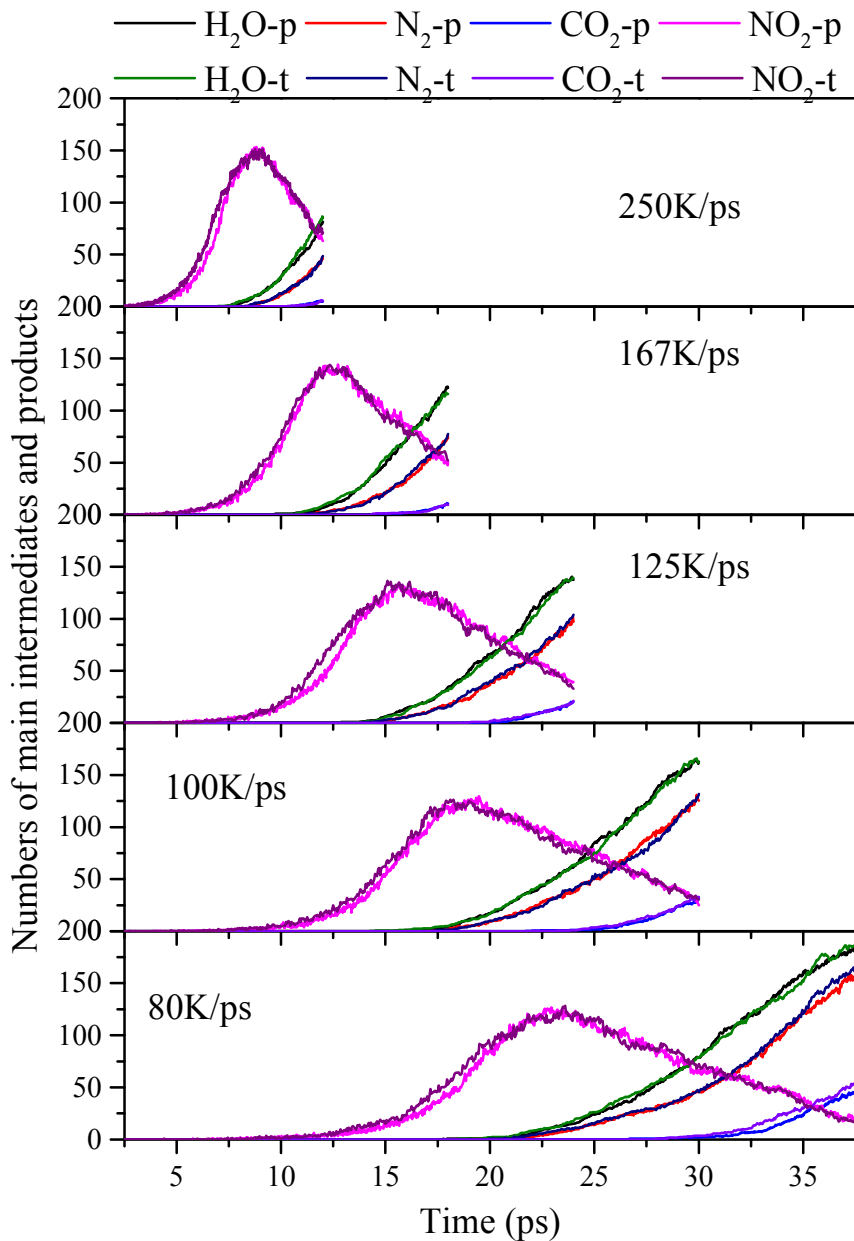

Figure s6. Evolution of the main intermediates and products during thermal decay of HMX.
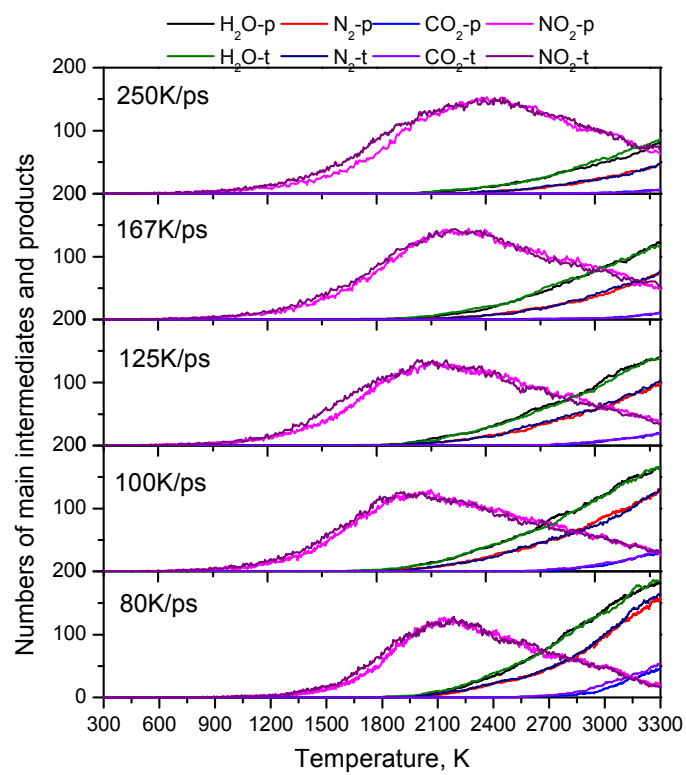
Figure s7. The evolution of the main intermediates and products versus temperature.

S5. Evolution of the main intermediates and products during thermal decay of HMX under adiabatic heating conditions.
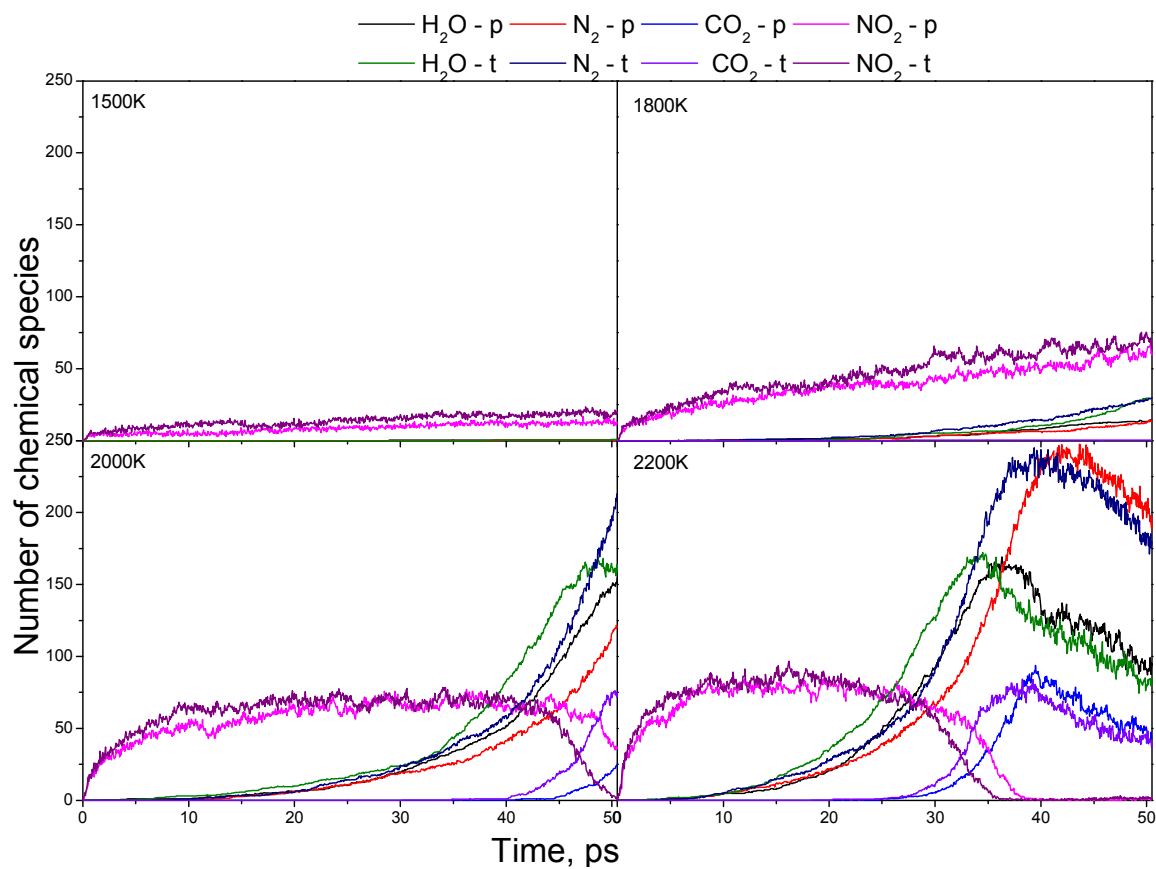

Figure s8. Evolution of main intermediates and products.

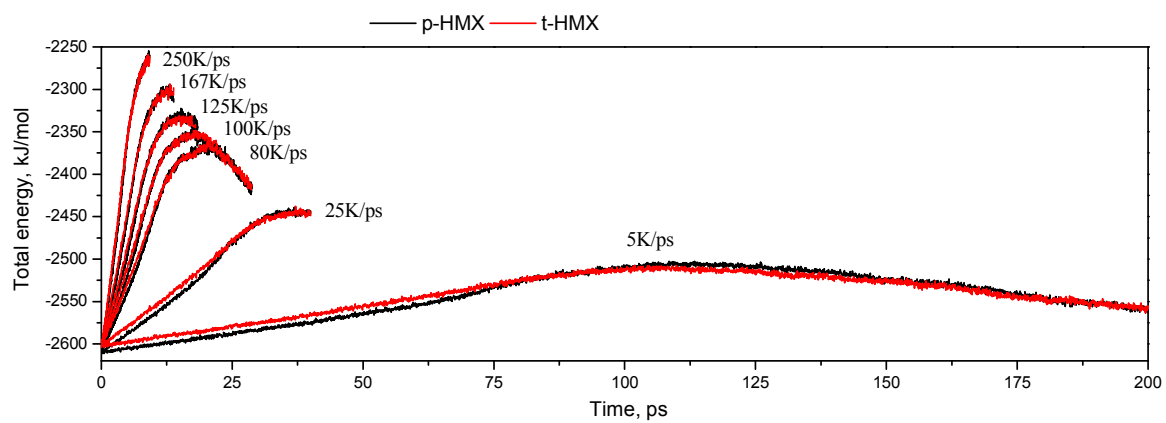## S6. Evolution of total energy of HMX under programmed heating conditions.

Figure s9. Evolution of total energy of HMX under programmed heating conditions.

S7. Rough calculations of heat input rates.

The total energies of the programmed heating model were normalized by the numbers of the HMX molecules. The heat input rates from environment were calculated from the linear fitting of the total energy curve. Considering the influence of the reaction on the total energy, the earlier stage (about the first 40%~50%) of the computing time was taken out to analyze. Similar processes were applied to the constant temperature heating processes to get the heat input rates of the constant temperature heating model, but the time taken out was much shorter, only the initial sharply raising stage (about 0.02 to 0.14ps) was adopted.