Supporting Information

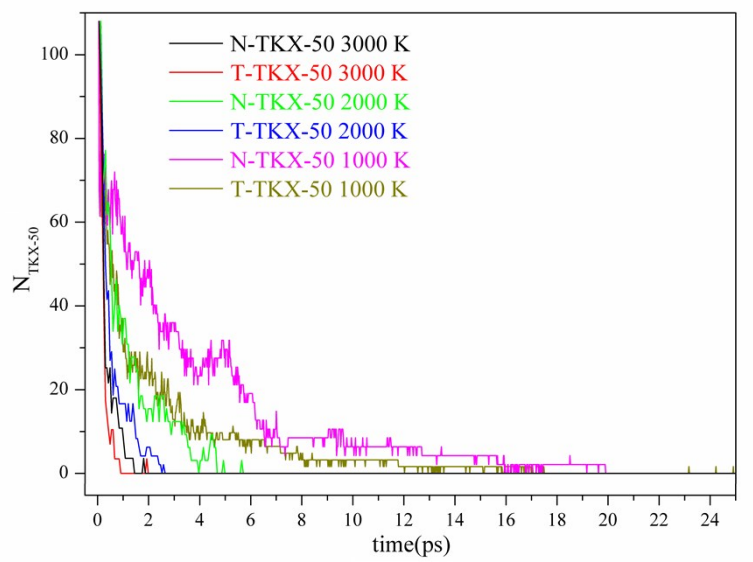


Fig. 1 Evolution of the amounts of TKX-50 molecules.

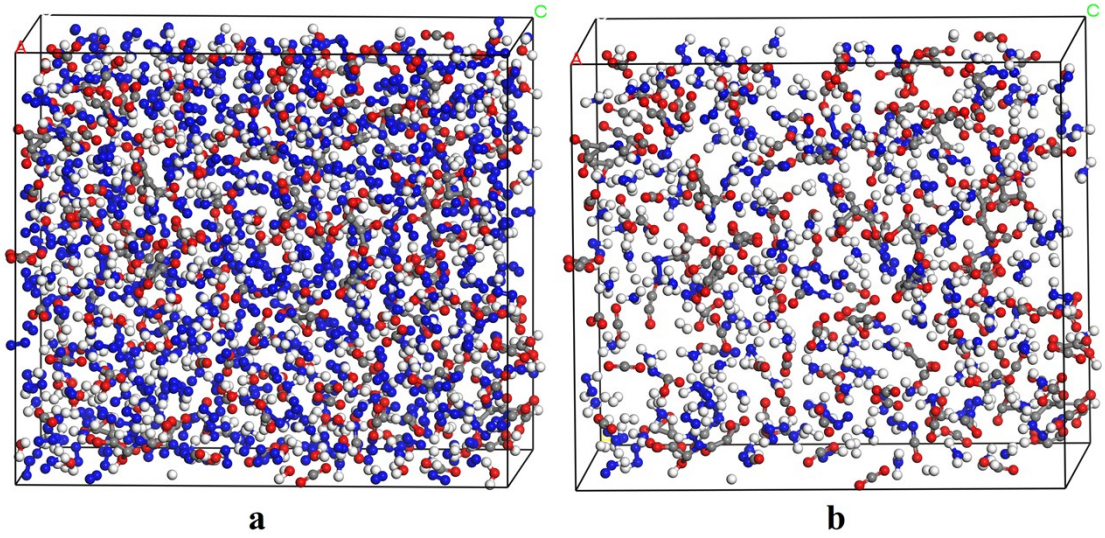


Fig. 2 Final configuration of the decomposition products of T-TKX-50.

The simulation results show that there are no TKX-50 or unstable intermediates after 200 ps simulation. All of the products are stable and small molecular products, such as H_2O, CO_2, N_2, NO, NO_2 and so on.

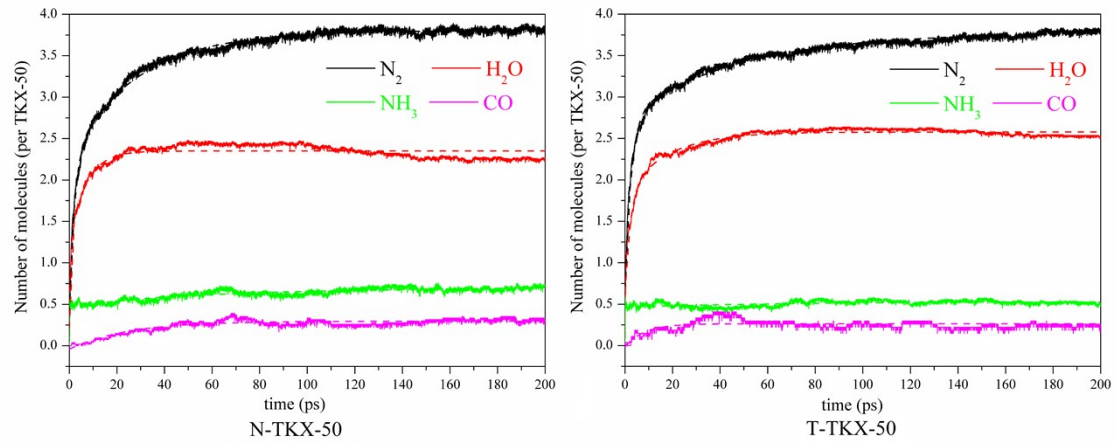


Fig. 3 Evolutions of the numbers of N_2, H_2O, NH_3 and CO molecules (solid lines) and their corresponding fitted curves (dash lines) of N-TKX-50 and T-TKX-50 at 2000 K.

As seen in Fig. 3, there is an excellent agreement between the simulation and fitting amounts of all measured end-products.

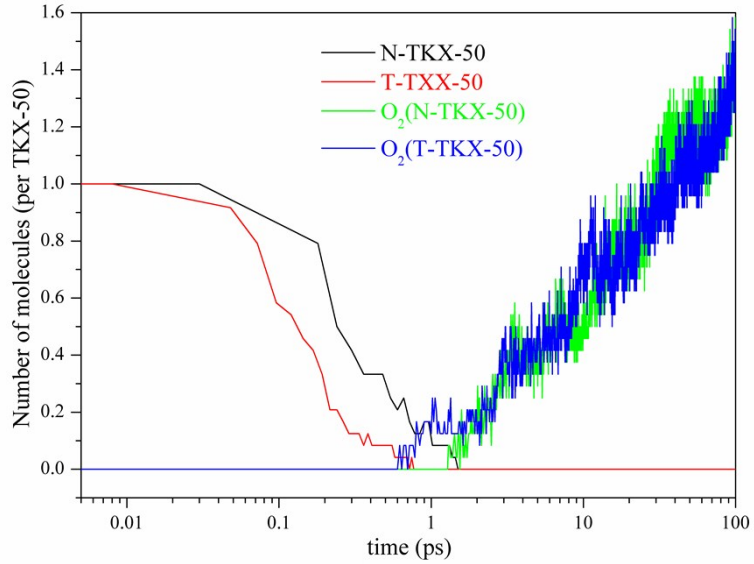
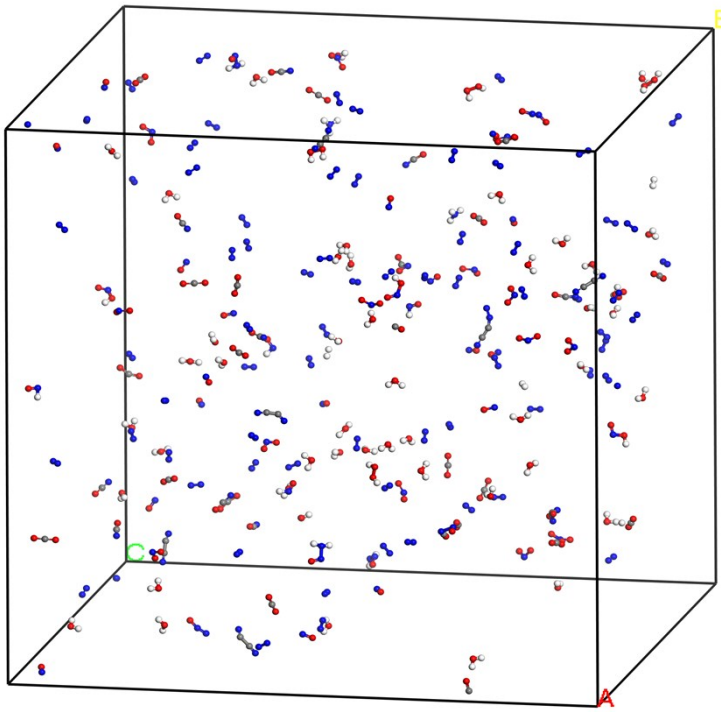


Fig. 4 TKX-50 distribution and consumption rate of O_2

Fig. 4 illustrates that the consumption rate of N-TKX-50 is slower than that of T-TKX-50 at the same temperature, demonstrating that T-TKX-50 combusts faster than N-TKX-50. In addition, in the initial stage, the amount of O_2 maintain constant while the amount of N-TKX-50 and T-TKX-50 gradually decrease to 0. This phenomenon demonstrates the hydroxylamine and bistetrazole ions of TKX-50 do not react with O_2 directly.



T-TKX-50

Fig. 5 Final configuration of the oxidation products of T-TKX-50.

It can be concluded from Fig. 5 that there is no existence of TKX-50 or unstable intermedia products after 500 ps simulation. All of the products are stable small molecular products, such as H_2O, CO_2, N_2, NO, NO_2 and so on.