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Supporting Information

Molecular dynamics study on the effect of metal ion doping on the performance of HMX

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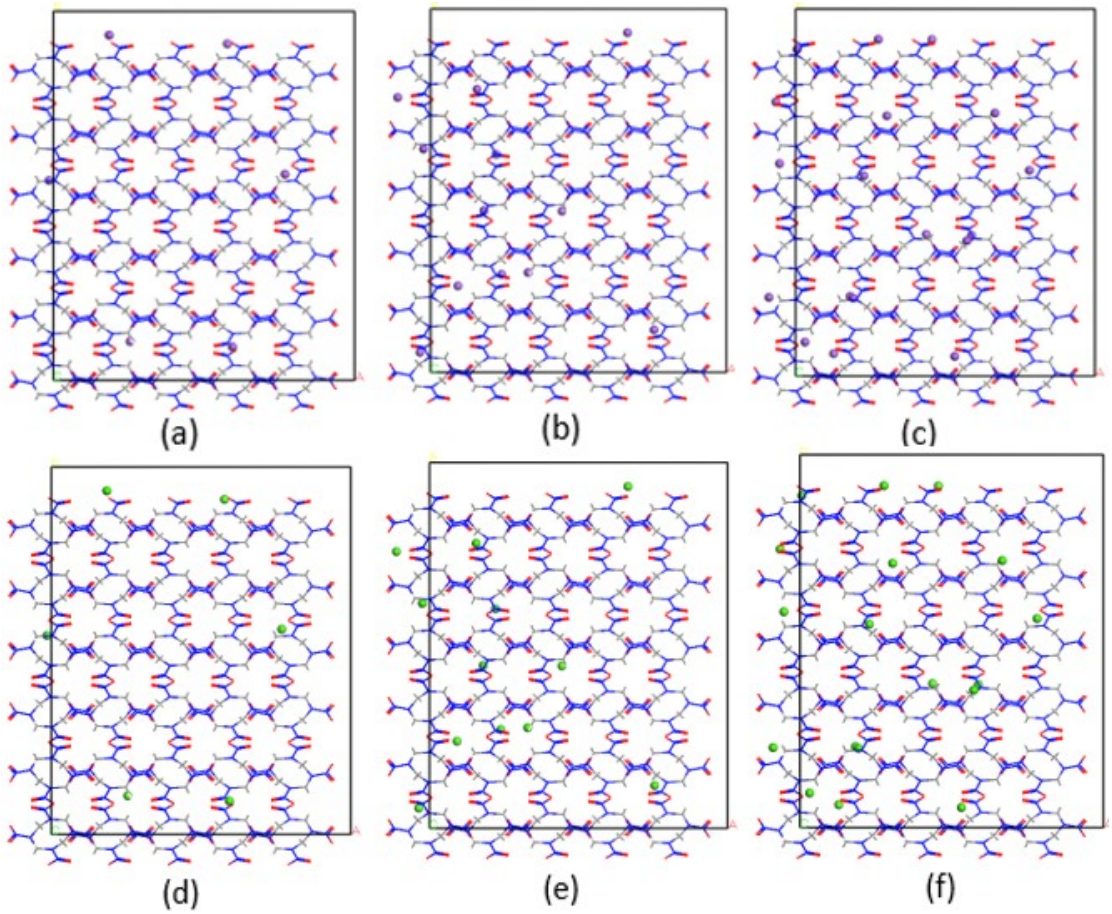

Figure S1. The position of doped metal ions in the HMX supercell model. (a), (b) and (c) represent 6,12 and 18 na^{+} doped in the HMX supercell model, respectively. (d), (e) and (f) represent 6,12 and 18 ca^{2+} doped in the HMX supercell model, respectively.

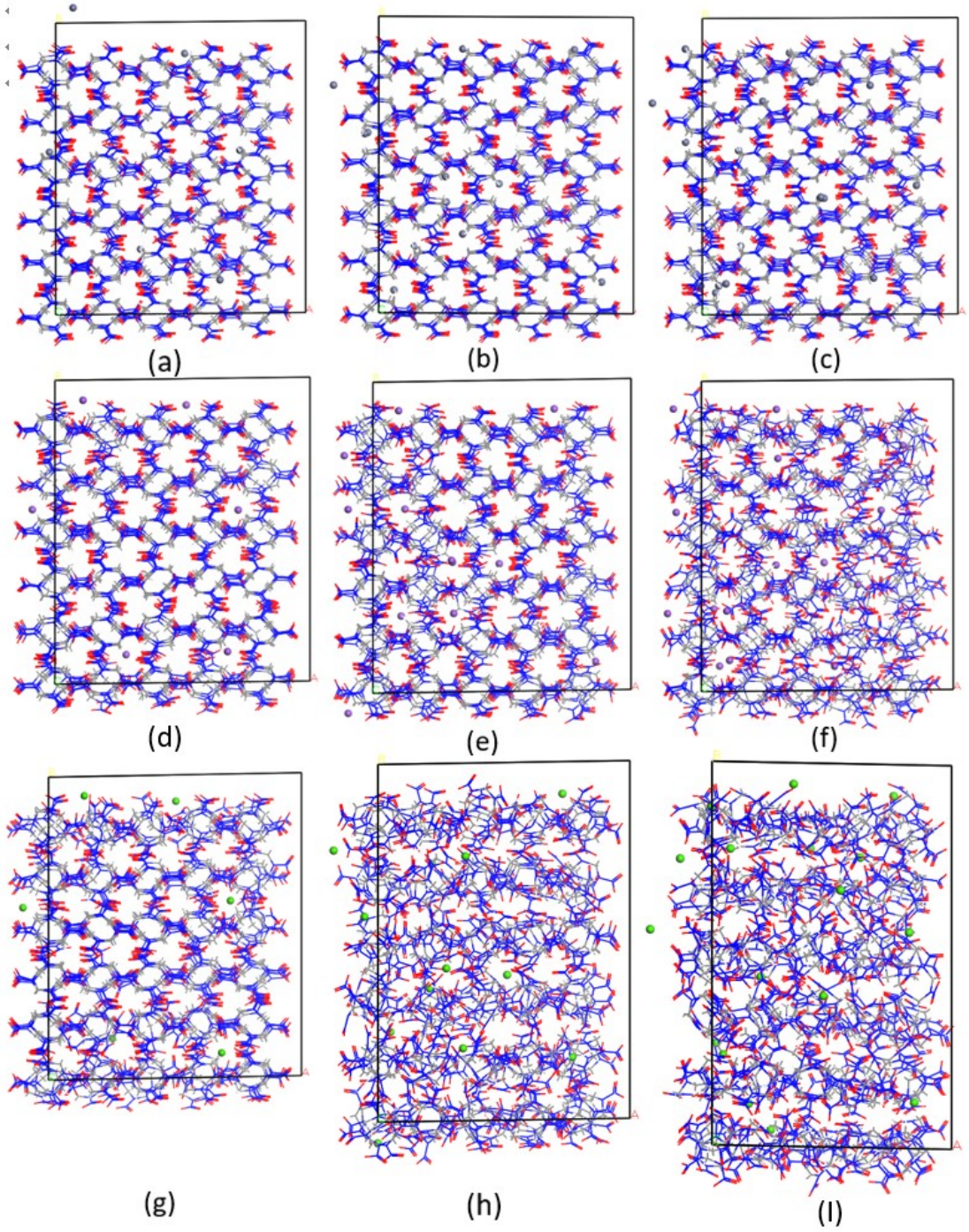

Figure S2. The equilibrium structure of the defect model. (a), (b) and (c) represent 6,12 and 18 zn^{2+} doped in the HMX supercell model, respectively. (d), (e) and (f) represent 6,12 and 18 na^{+} doped in the HMX supercell model, respectively. (g), (h) and (I) represent 6,12 and 18 ca^{2+} doped in the HMX supercell model, respectively.

Table S1 The energy of the model in the equilibrium state

n(Model)	1	2	3	4	5	6	7	8	9	10
$E_1(kJ/mol)$	-120193	-120145	-120757	-122306	-121878	-123747	-126123	-127003	-135460	-145151
$E_2(kJ/mol)$	-27527	-28011	-28217	-29799	-29828	-32901	-37739	-37588	-50340	-62105

E_1 represents the total energy of the system in the equilibrium state; E_2 represents the total energy of the model system after all the N atoms in the explosive are fixed in the equilibrium state. As illustrated in Figure S2. The energy of the zinc ion doping defect model falls while it increases for the sodium ion and calcium ion doping models. It demonstrates that zinc ion doping has no effect on the total energy of HMX; the more flaws there are, the more noticeable the total energy increase caused by calcium ion doping.

The total energy of the system reduces dramatically once the N atom is fixed, demonstrating that the energy in HMX is mostly provided by the N atom, and hence the energy of the N-N bond would directly affect the HMX sensitivity.