

Supplementary Information

The effects of nonmetal dopants on the electronic, optical and catalytic performances of monolayer WSe₂ by first-principles study

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Fig. 1S The schematic diagram of specimens including and excluding the dopant, (a) substituted specimen, (b) interstitial specimen and (c) specimen excluding a dopant with a vacancy

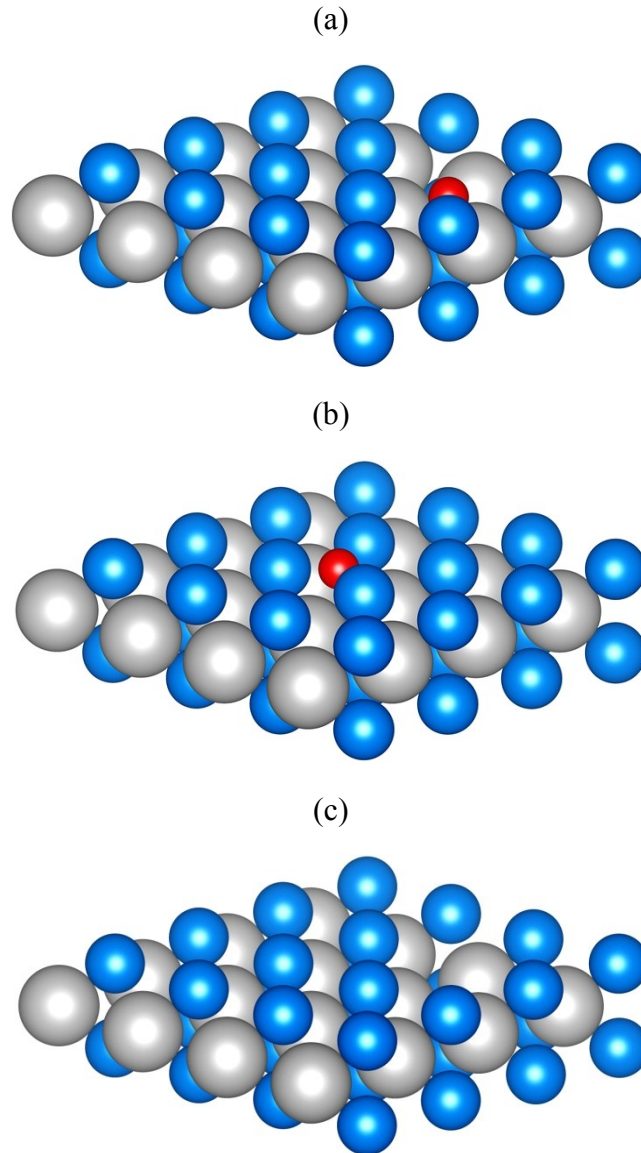
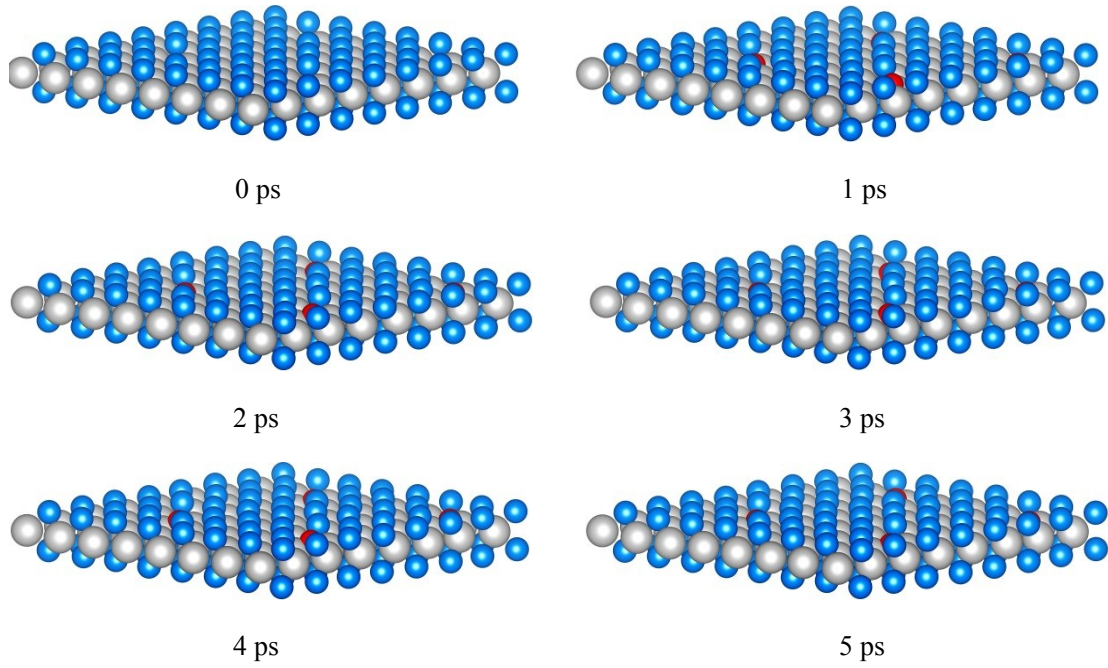
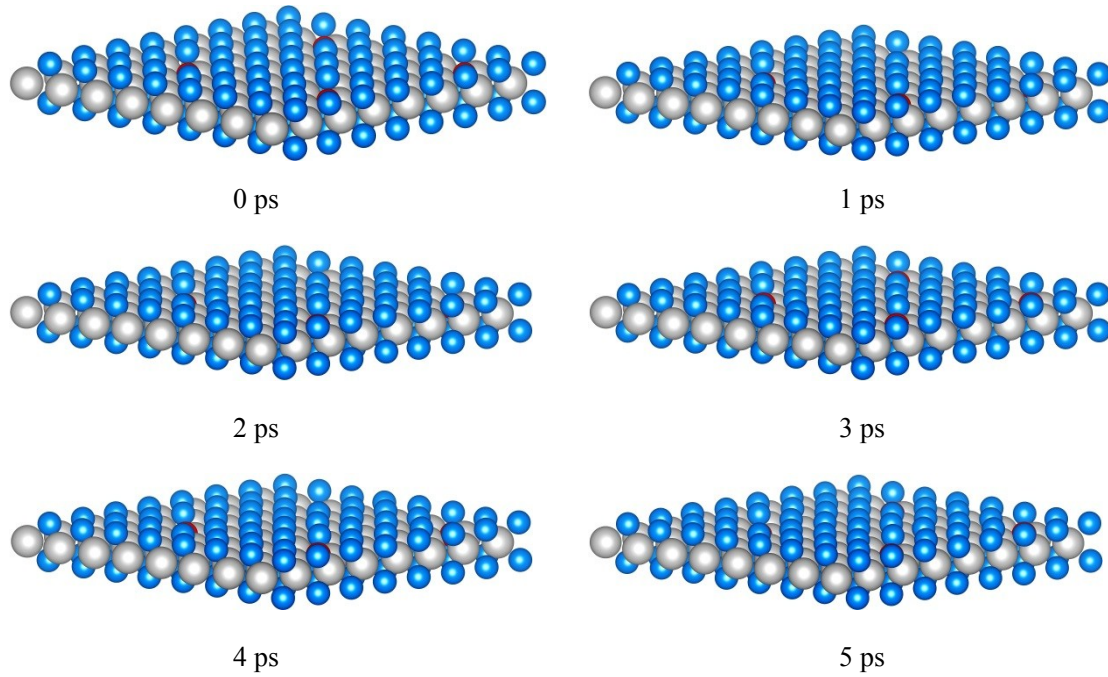


Fig. 2S The configurations of substituted WSe₂ at 0, 1, 2, 3, 4 and 5 ps.

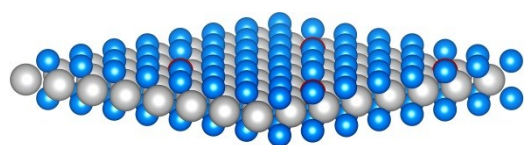
(a) H doped



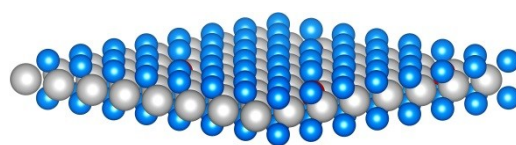
(b) B doped



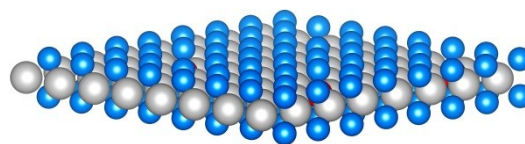
(c) C doped



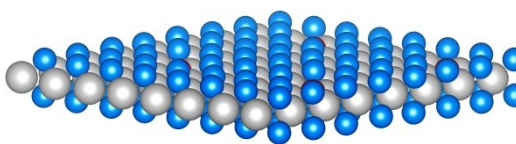
0 ps



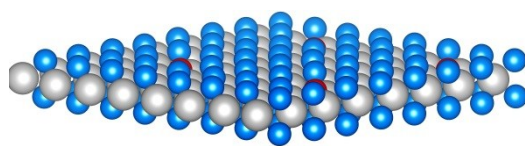
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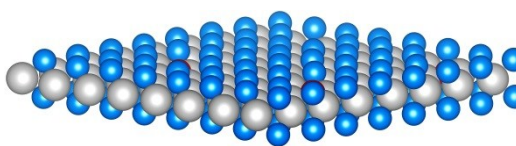
2 ps



3 ps

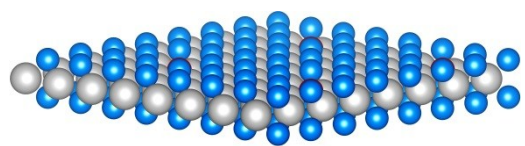


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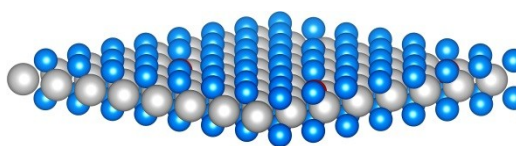


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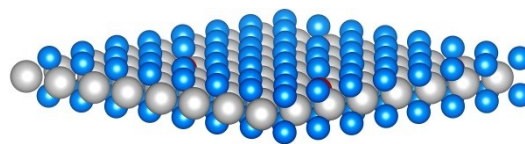
(d) N doped



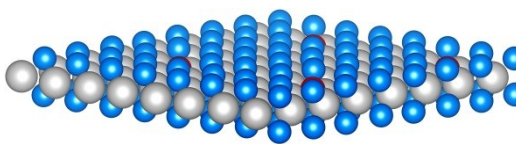
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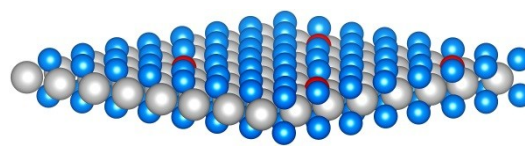
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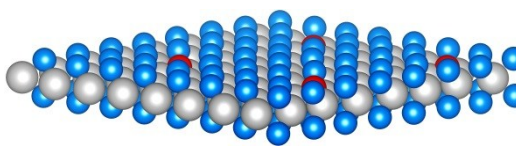
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3 ps



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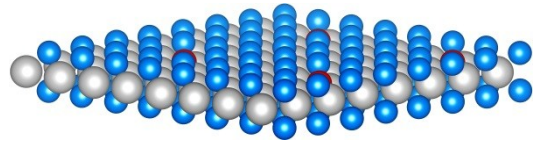


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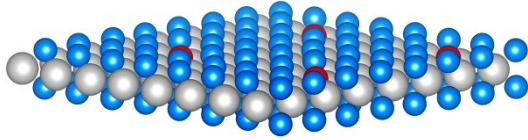
(e) O doped



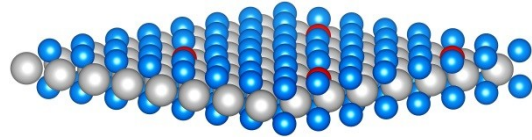
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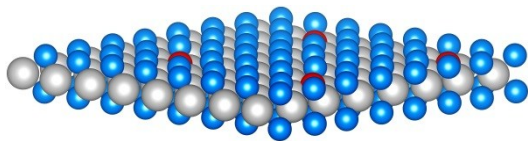
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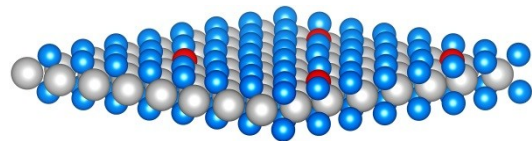
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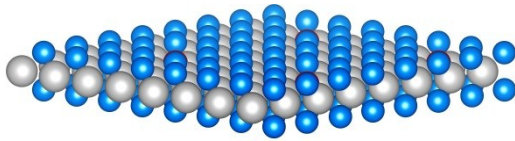


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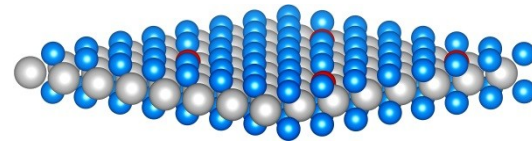


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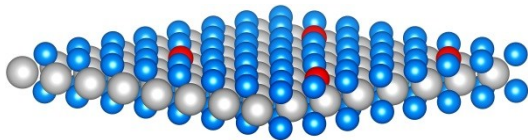
(f) F doped



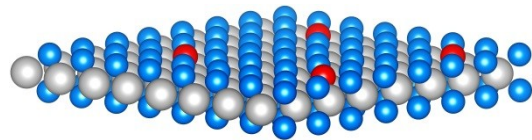
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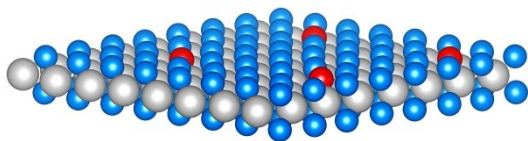
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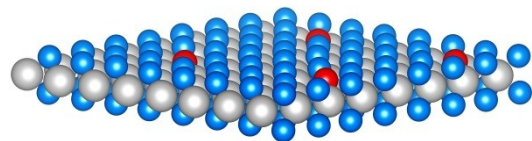
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3 ps

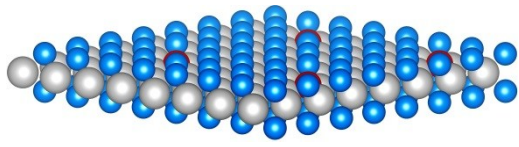


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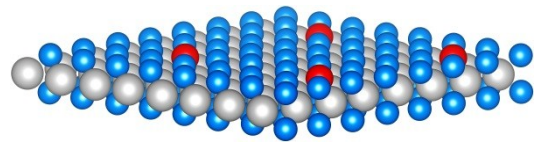


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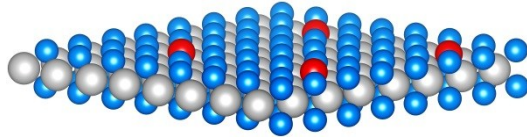
(g) Si doped



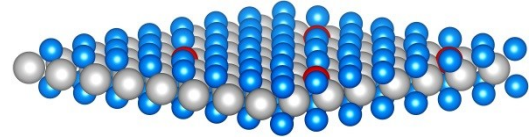
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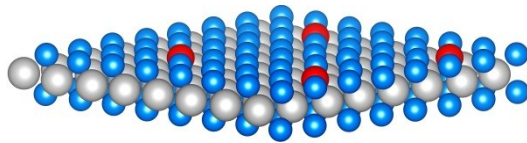
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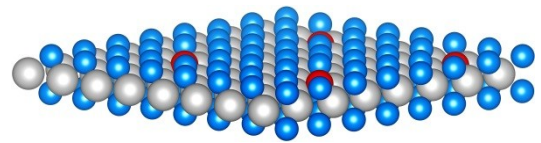
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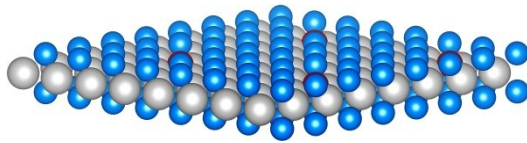


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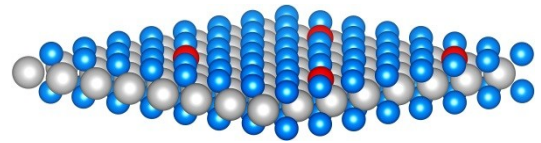


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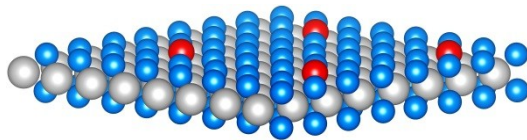
(h) P doped



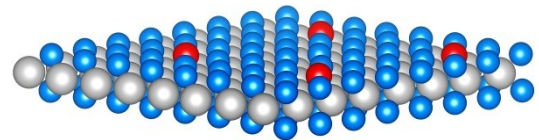
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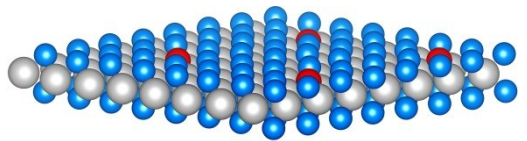
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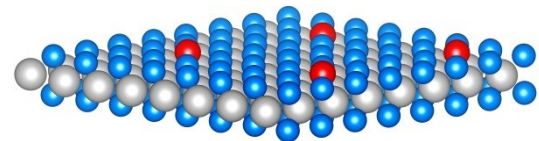
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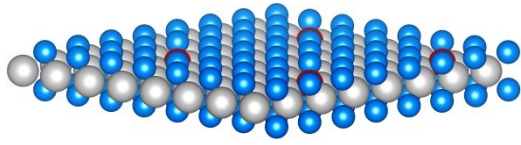


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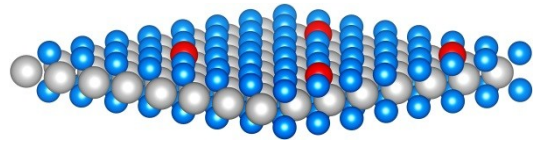


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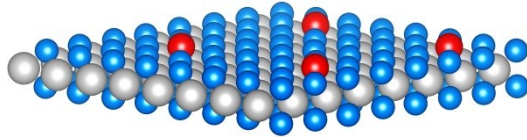
(i) S doped



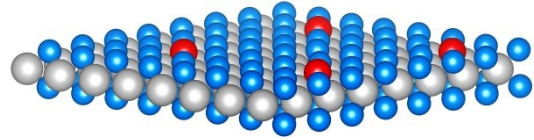
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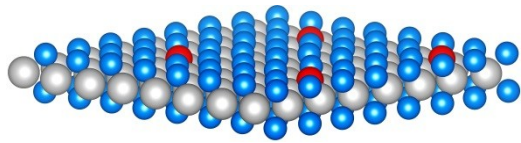
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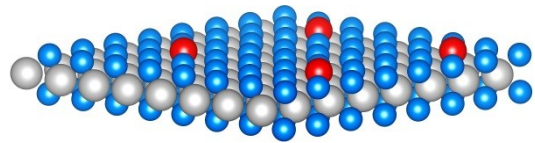
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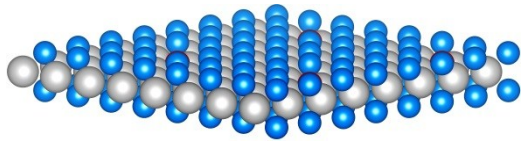


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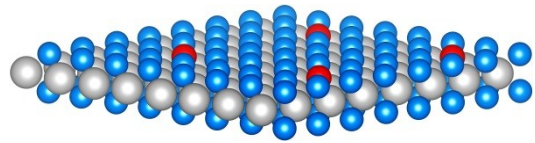


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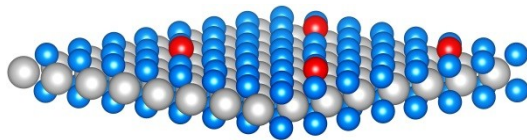
(j) Cl doped



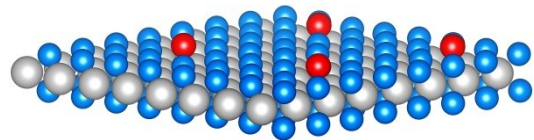
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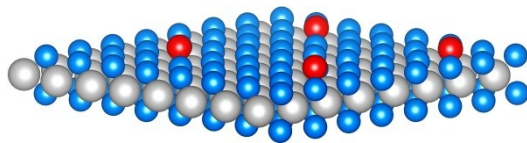
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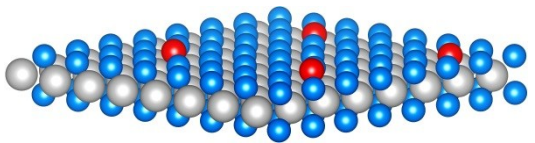
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3 ps

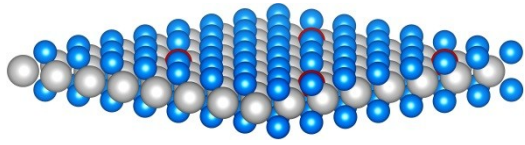


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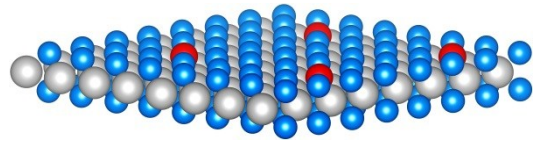


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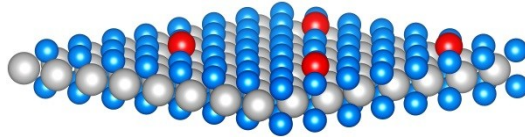
(k) As doped



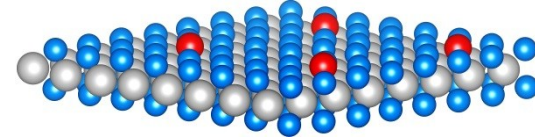
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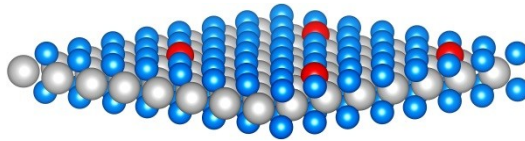
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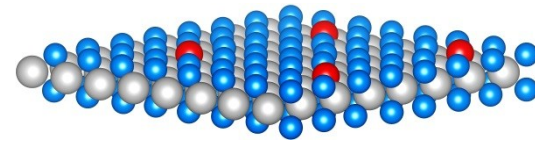
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3 ps

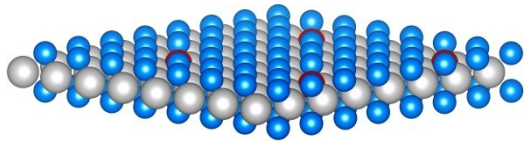


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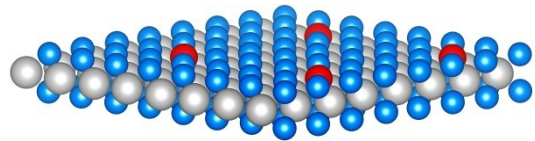


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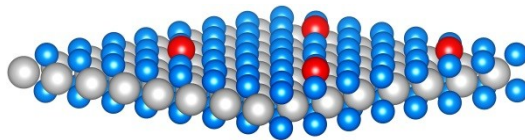
(l) Br doped



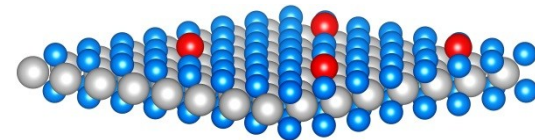
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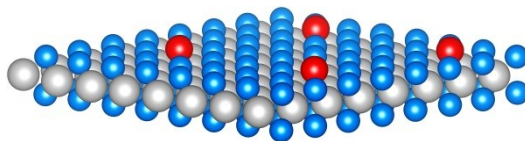
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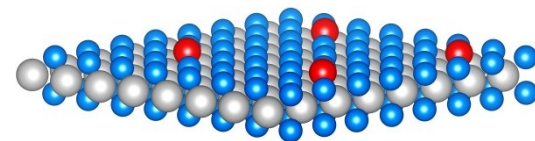
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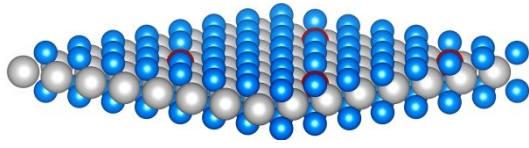


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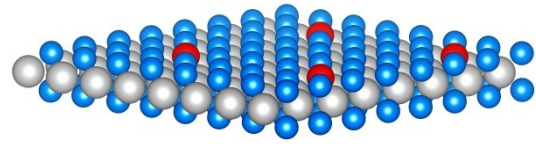


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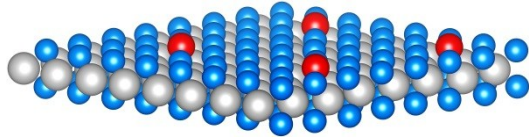
(m) Te doped



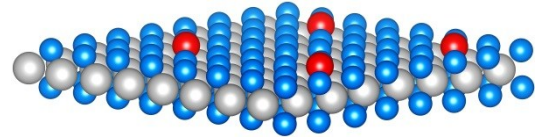
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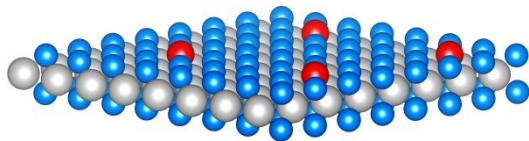
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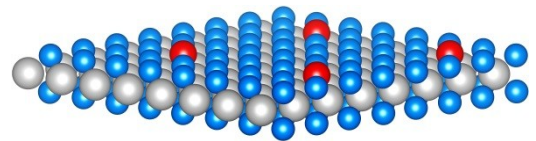
2 ps



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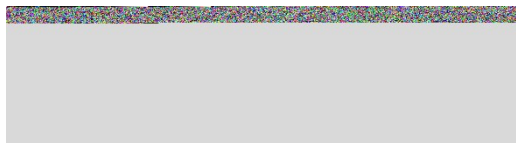


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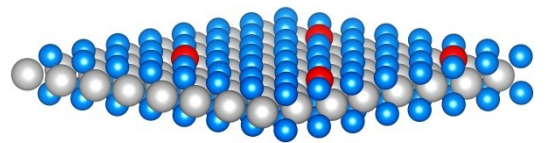


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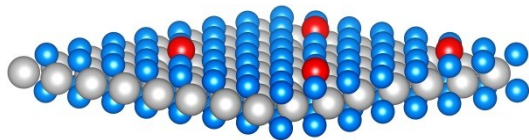
(n) I doped



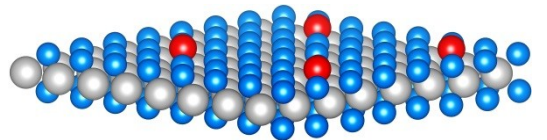
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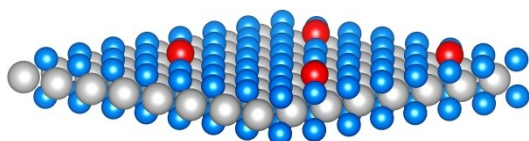
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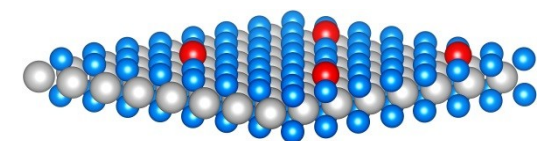
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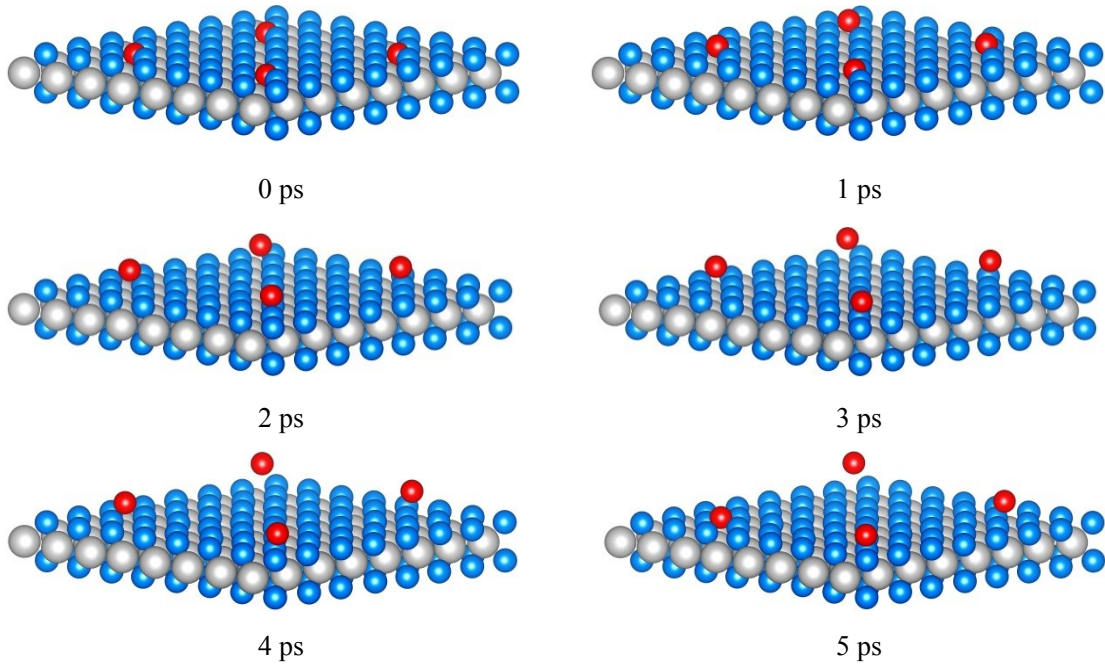
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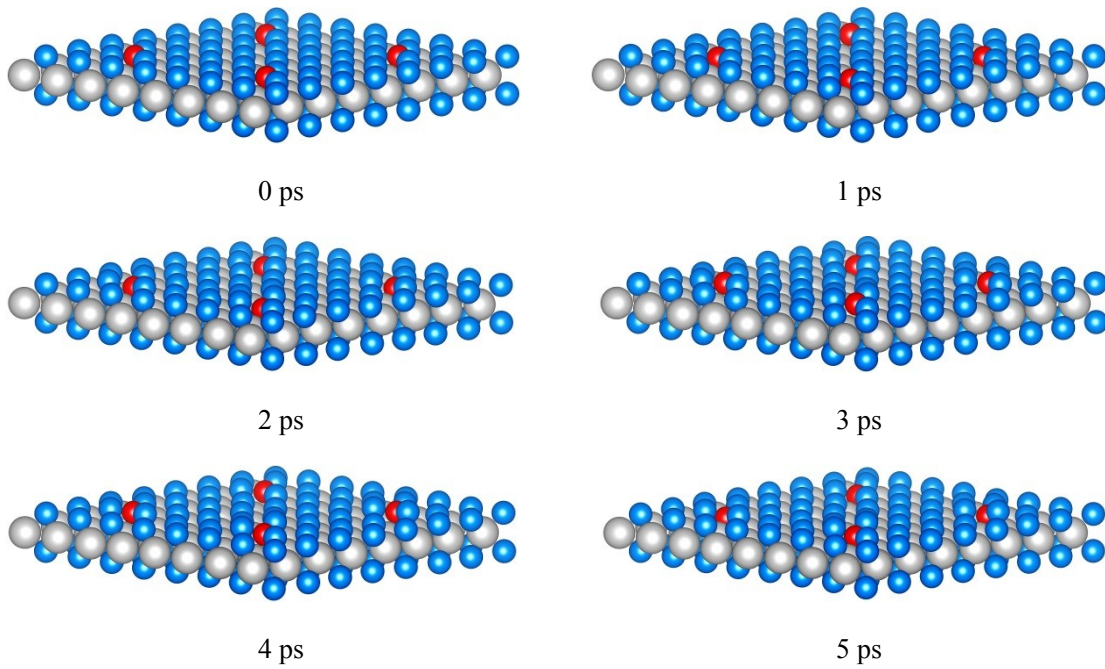
5 ps

Fig. 3S The configurations of interstitial WSe₂ at 0, 1, 2, 3, 4 and 5 ps.

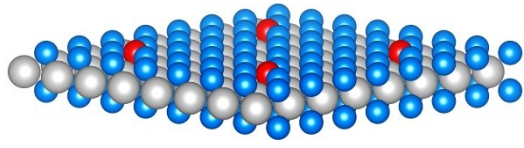
(a) H doped



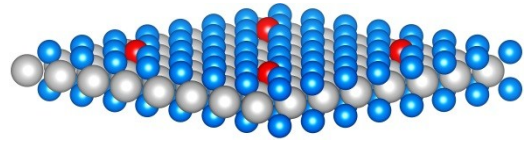
(b) B doped



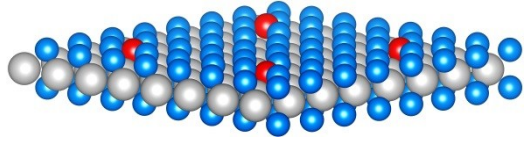
(c) C doped



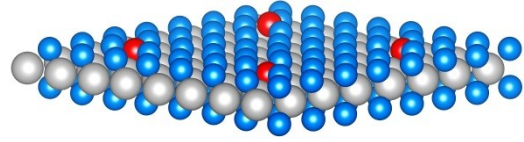
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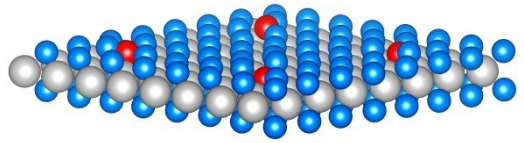
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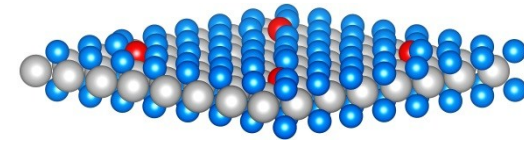
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3 ps

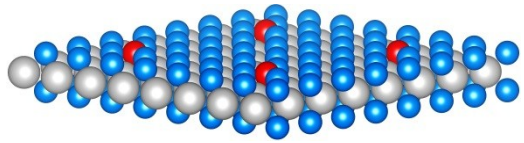


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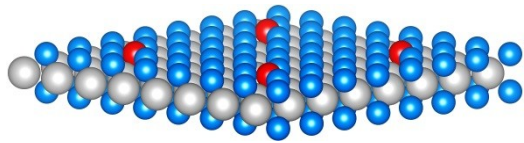


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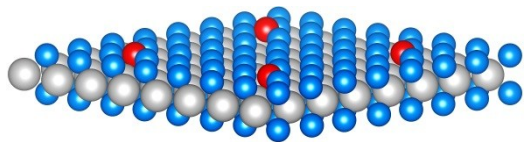
(d) N doped



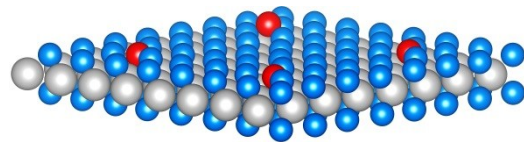
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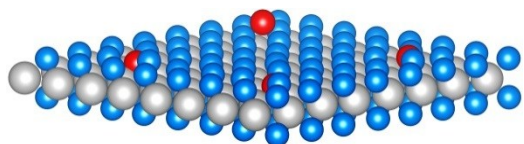
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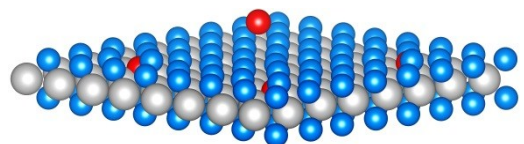
2 ps



3 ps

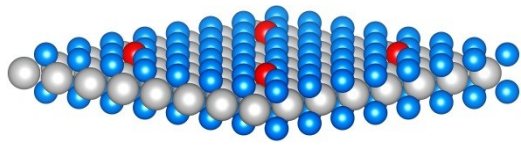


4 ps

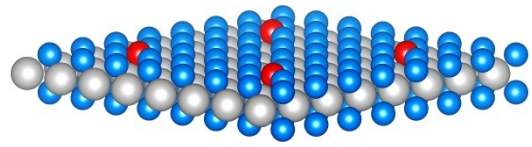


5 ps

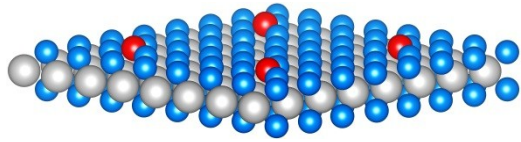
(e) O doped



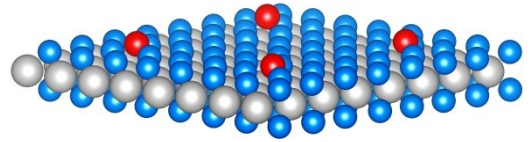
0 ps



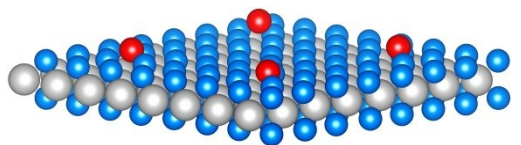
1 ps



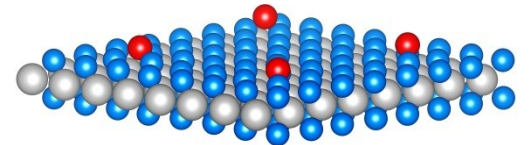
2 ps



3 ps

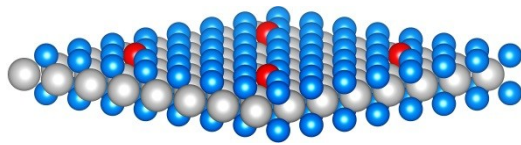


4 ps

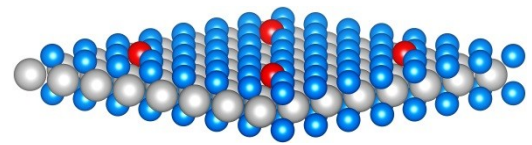


5 ps

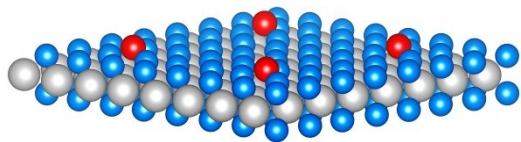
(f) F doped



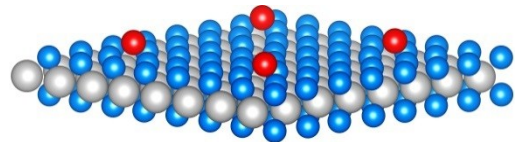
0 ps



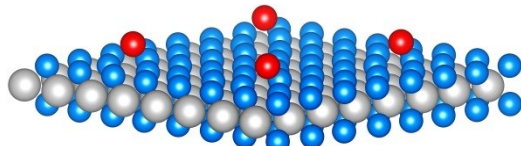
1 ps



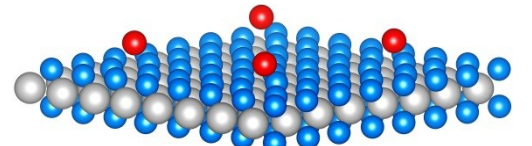
2 ps



3 ps

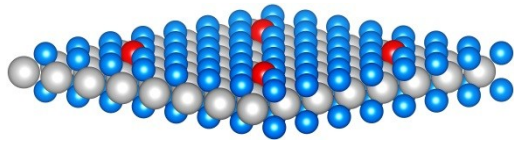


4 ps

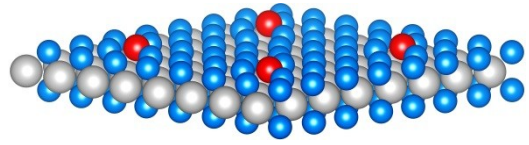


5 ps

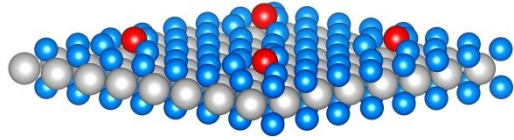
(g) Si doped



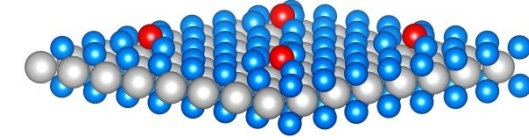
0 ps



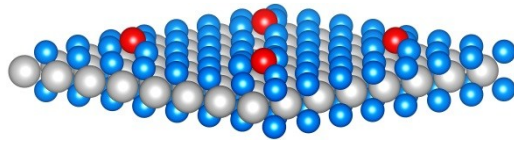
1 ps



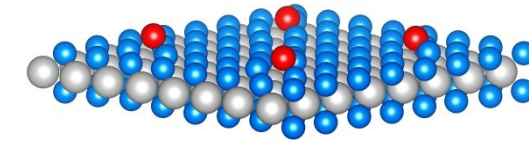
2 ps



3 ps

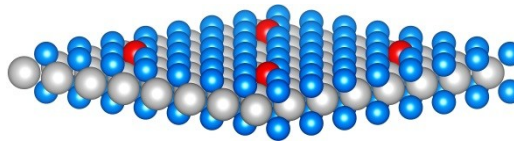


4 ps

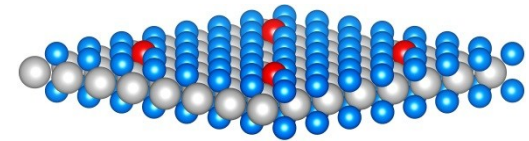


5 ps

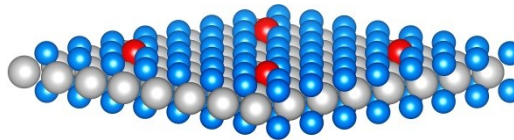
(h) P doped



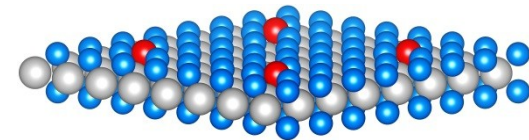
0 ps



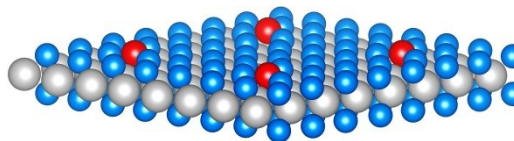
1 ps



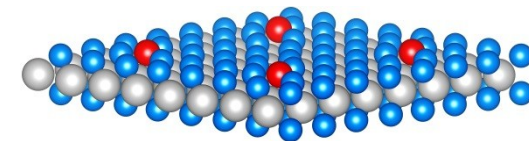
2 ps



3 ps

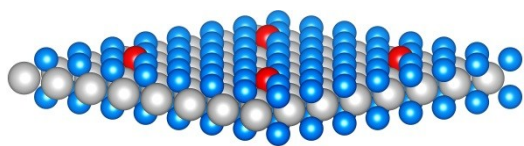


4 ps

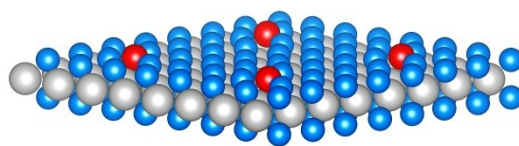


5 ps

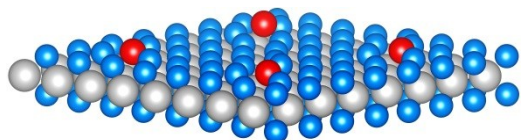
(i) S doped



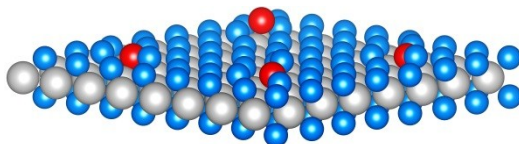
0 ps



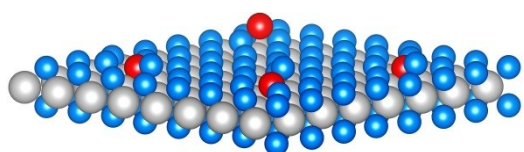
1 ps



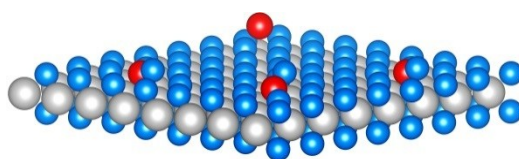
2 ps



3 ps

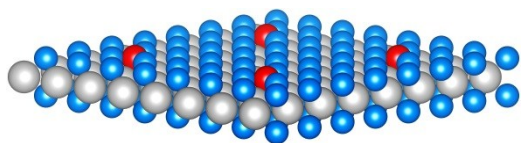


4 ps

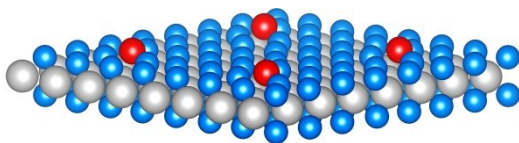


5 ps

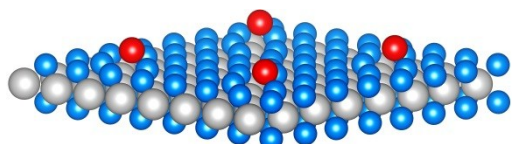
(j) Cl doped



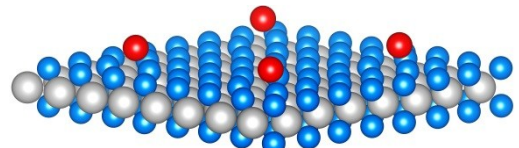
0 ps



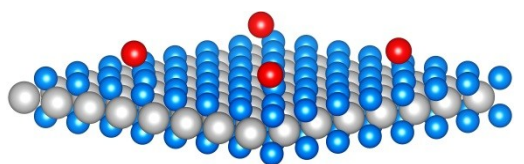
1 ps



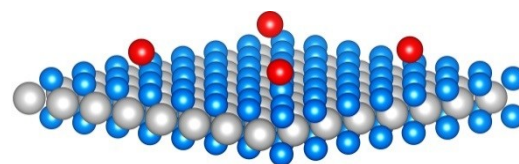
2 ps



3 ps

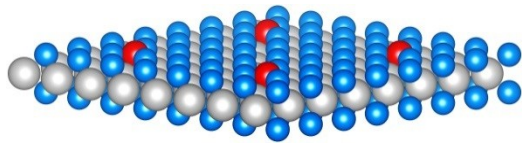


4 ps

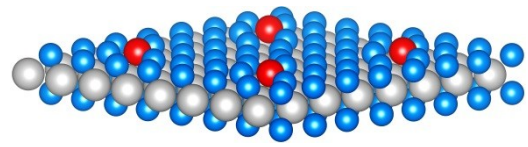


5 ps

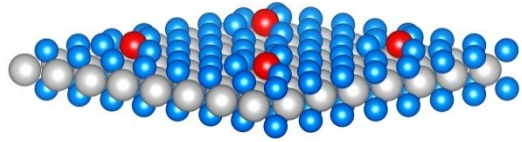
(k) As doped



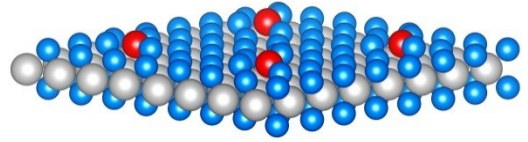
0 ps



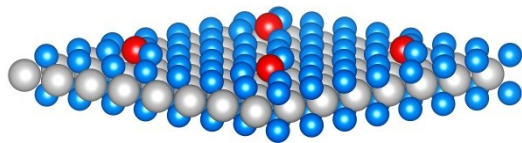
1 ps



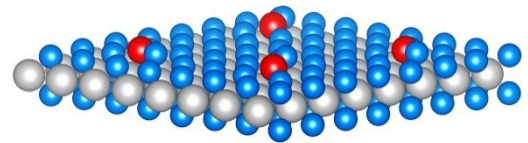
2 ps



3 ps

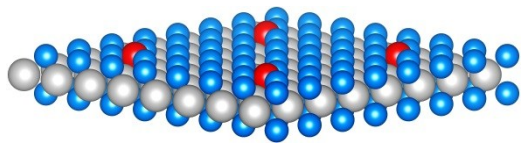


4 ps

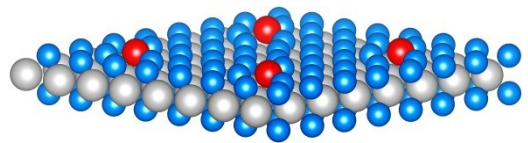


5 ps

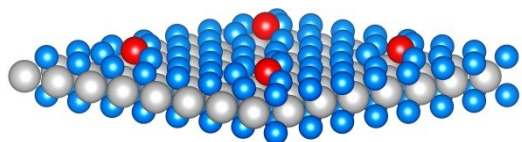
(l) Br doped



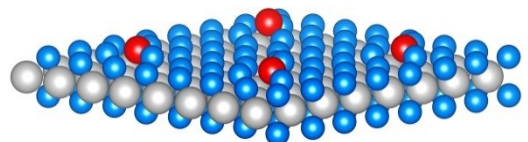
0 ps



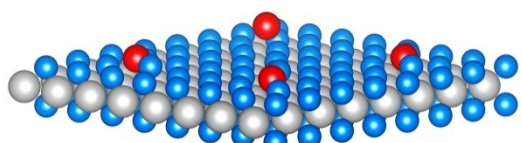
1 ps



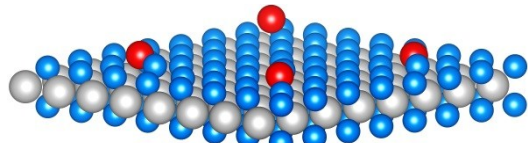
2 ps



3 ps

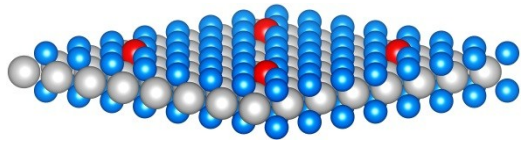


4 ps

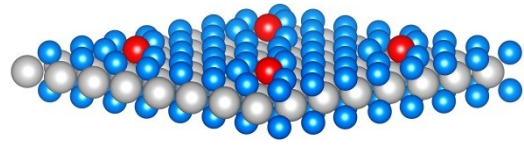


5 ps

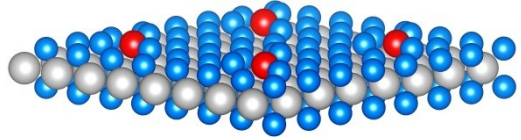
(m) Te doped



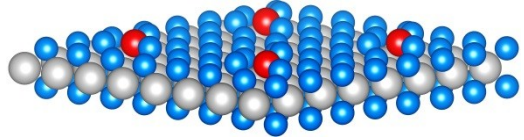
0 ps



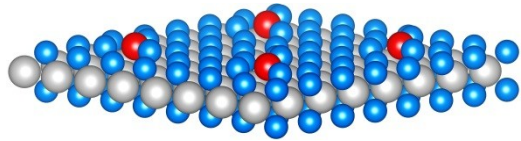
1 ps



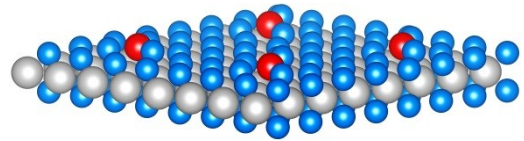
2 ps



3 ps

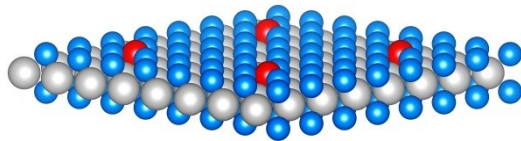


4 ps

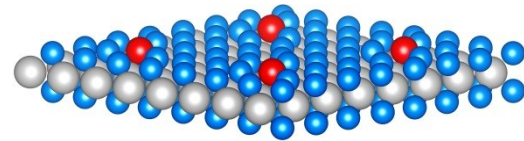


5 ps

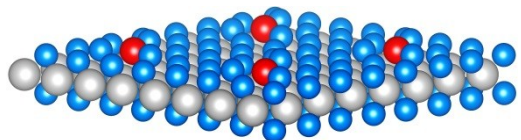
(n) I doped



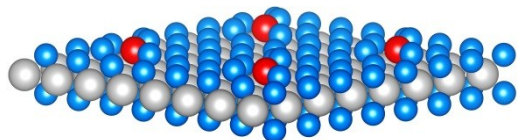
0 ps



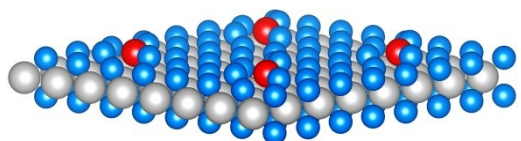
1 ps



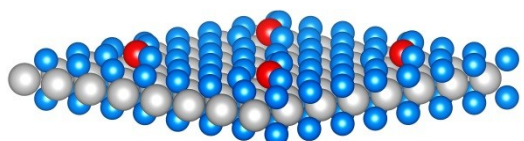
2 ps



3 ps



4 ps



5 ps