Figure S1. The PBE+U optimized structure of the (a) pristine $Ti_3C_2O_2$ MXene surface, (b) oxygen-deficient $Ti_3C_2O_2$ surface, showing the bond lengths of the defected surface (the dotted red line indicates the removed O atom from the surface), (c) free H_2O_2 molecule, (d) adsorbed H_2O_2 on the pristine $Ti_3C_2O_2$ surface (the inset shows the distortion of the H–O–O–H dihedral angle), and (e) adsorbed/dissociated H_2O_2 on the oxygen-deficient $Ti_3C_2O_2$ surface. Distances are given in angstroms (Å).

Figure S2. MLIP–MD equilibration and total energy evolution for H_2O_2 adsorption and dissociation on $Ti_3C_2O_2$–O_{vac}.
(a) Temperature and total energy profiles at 0 K showing rapid convergence and structural stabilization without O–O bond cleavage.
(b) Simulation at 300 K indicating thermal equilibration and a stepwise decrease in total energy associated with H_2O_2 activation and dissociation on the defective surface.
(c) Explicit aqueous simulation ($nH_2O + H_2O_2$) at 300 K demonstrating stable thermal fluctuations and a continuous decrease in total energy, reflecting enhanced reactivity and stabilization of reaction intermediates in water.

Figure S1.

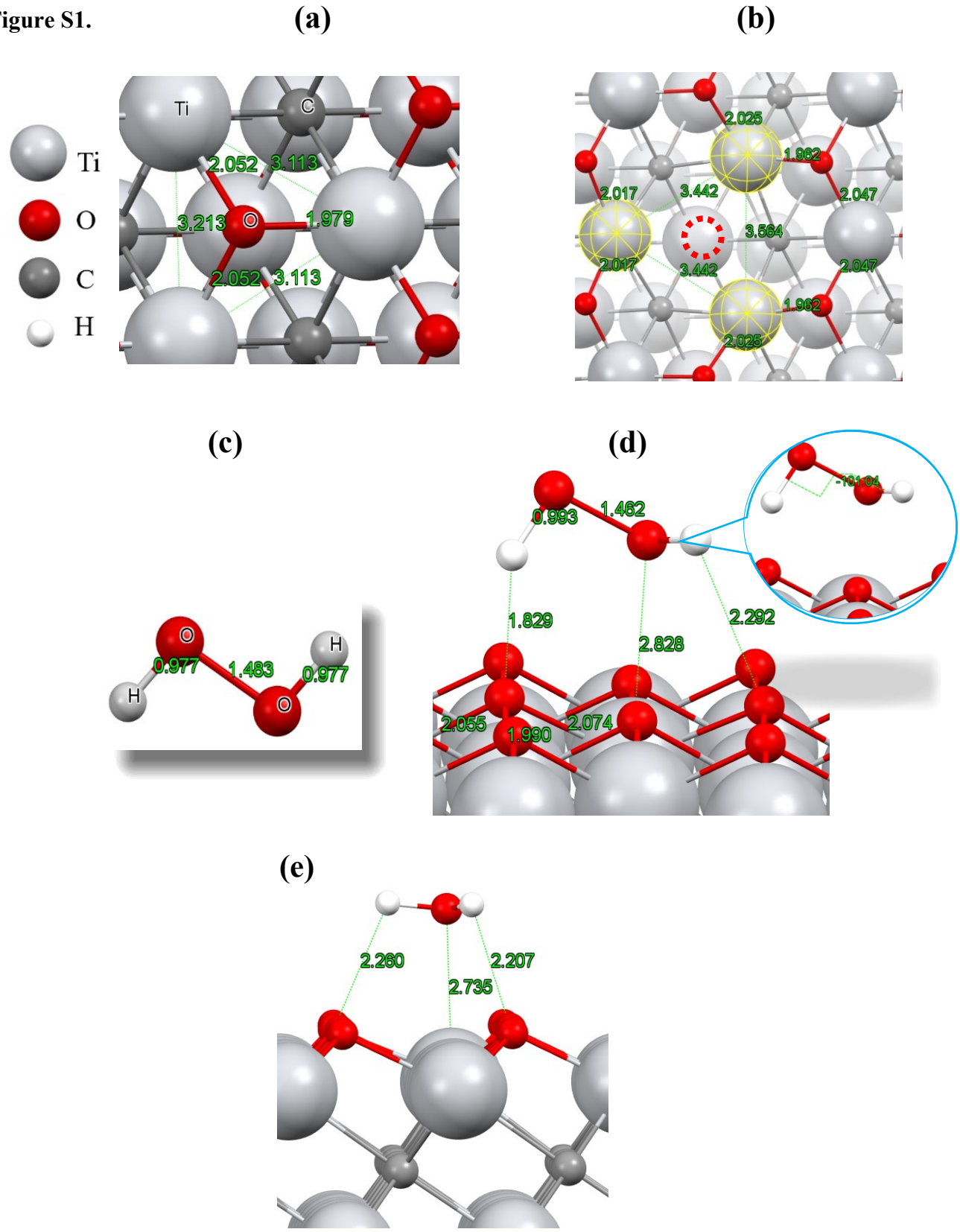
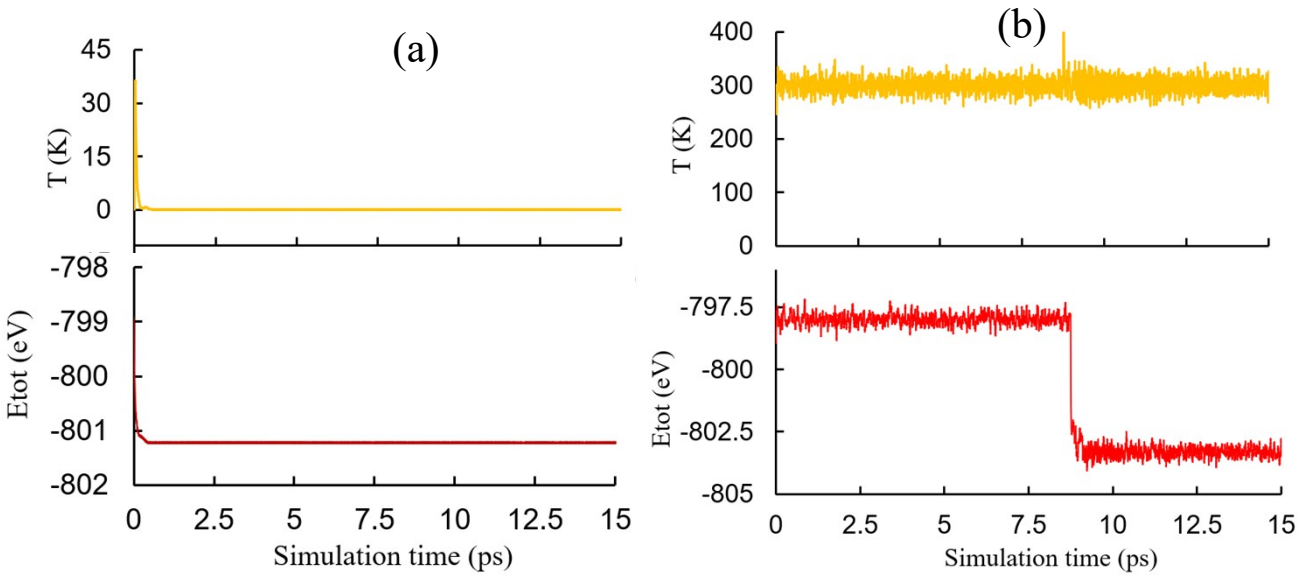
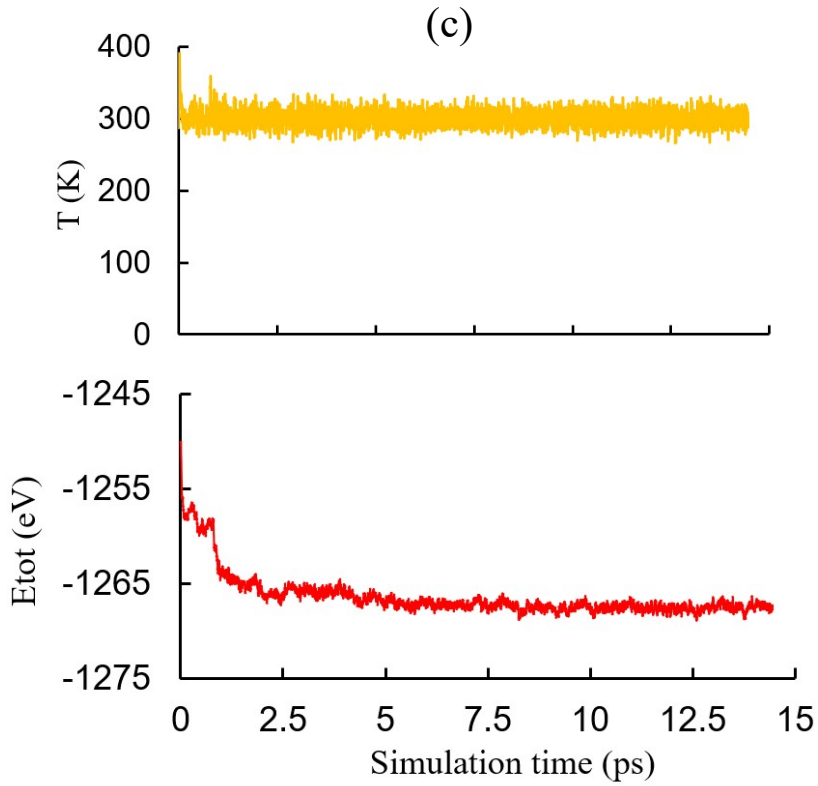

(a)
(b)
(c)
(d)
(e)
Ti
O
C
H
Ti
C
2.052
3.113
3.213
O
1.979
2.052
3.113
2.025
1.962
2.017
3.442
2.047
3.564
2.017
3.442
2.047
1.962
2.025
O
H
0.977
1.483
0.977
H
O
0.993
1.462
1.829
2.292
2.828
2.055
1.990
2.074
2.260
2.207
2.735

Figure S2


(a)
T (K)
45
30
15
0
Etot (eV)
-798
-799
-800
-801
-802
0
2.5
5
7.5
10
12.5
15
Simulation time (ps)
(b)
T (K)
400
300
200
100
0
Etot (eV)
-797.5
-800
-802.5
-805
0
2.5
5
7.5
10
12.5
15
Simulation time (ps)


(c)
T (K)
400
300
200
100
0
Etot (eV)
-1245
-1255
-1265
-1275
0
2.5
5
7.5
10
12.5
15
Simulation time (ps)