Supporting Materials
for

Adsorption and Dissociation of H_2O on W(111) surface : A Computational Study

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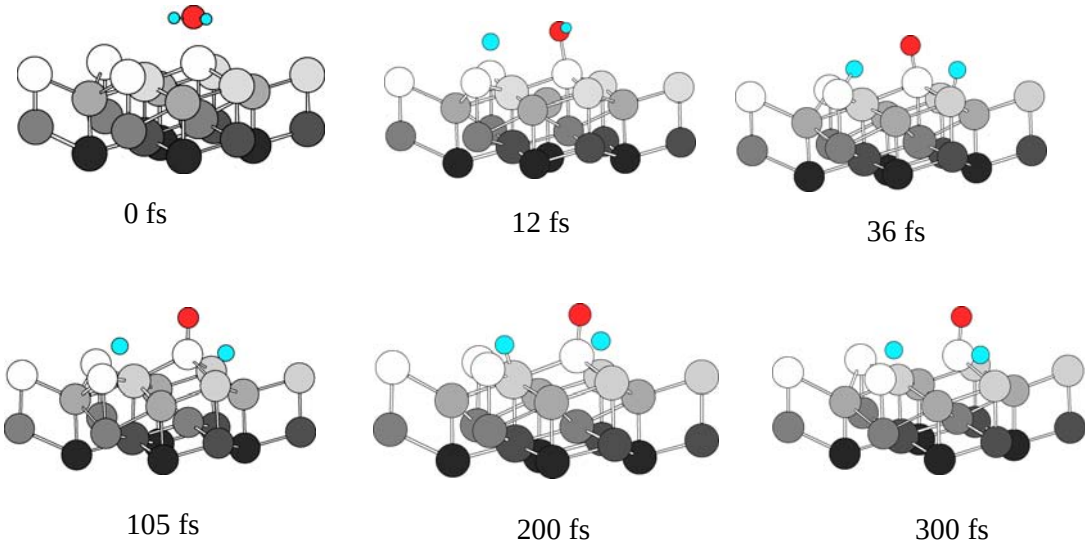
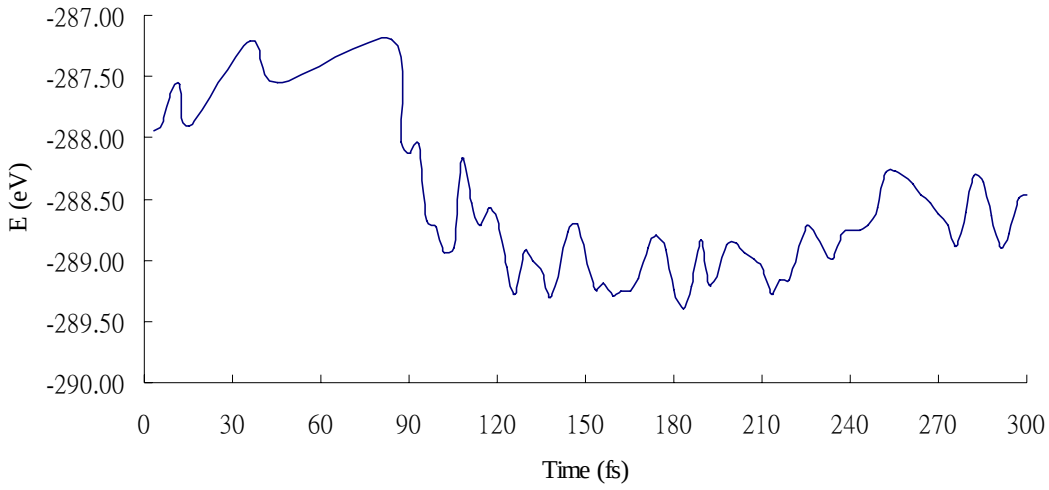
Table S1. The adsorption energies (kcal/mol) and geometry parameters for H_2O clusters on (2×2) and (3×3)-W(111) surface calculated at the rPBE level.

Cluster	$E_{(a)}$[a]	$d_{O\text{-}W}$	$d_{O\text{-}H1}$	$d_{O\text{-}H2}$	HOH	$d_{O\text{-}O}$
2×2-(111)						
Monomer	-12.6	2.308	0.985	0.983	105.3	
Dimer	-11.0	2.327	0.981	0.978	106.2	4.076
		2.345	0.983	0.983	104.9	
Trimer	-10.4	2.434	0.984	0.977	106.2	3.371
		2.370	0.981	0.975	107.0	3.487
		2.450	0.994	0.977	105.3	3.322
3×3-(111)						
Monomer	-12.4	2.305	0.979	0.979	106.9	
Dimer	-11.7	2.332	0.979	0.978	106.6	
		2.309	0.978	0.975	107.1	4.507
Trimer	-11.4	2.395	0.983	0.976	106.6	3.421
		2.363	0.980	0.976	106.7	3.350
		2.418	0.995	0.976	105.9	3.552
Hexamer	-11.9	2.363	0.982	0.979	105.0	3.446
		2.398	1.006	0.978	105.2	3.930
		2.361	0.981	0.977	106.5	4.108
		2.372	0.990	0.978	105.6	4.385
		2.356	0.984	0.980	104.6	4.490
		2.360	0.983	0.982	104.8	4.338

a. $E_{(a)} = (E[slab + [H_2O]n] – (E[slab] + n \times E[H_2O])/n$


0 fs
12 fs
36 fs
105 fs
200 fs
300 fs

(a)


-287.00
-287.50
-288.00
-288.50
-289.00
-289.50
-290.00
E (eV)
0
30
60
90
120
150
180
210
240
270
300
Time (fs)

(b)

Figure S1.