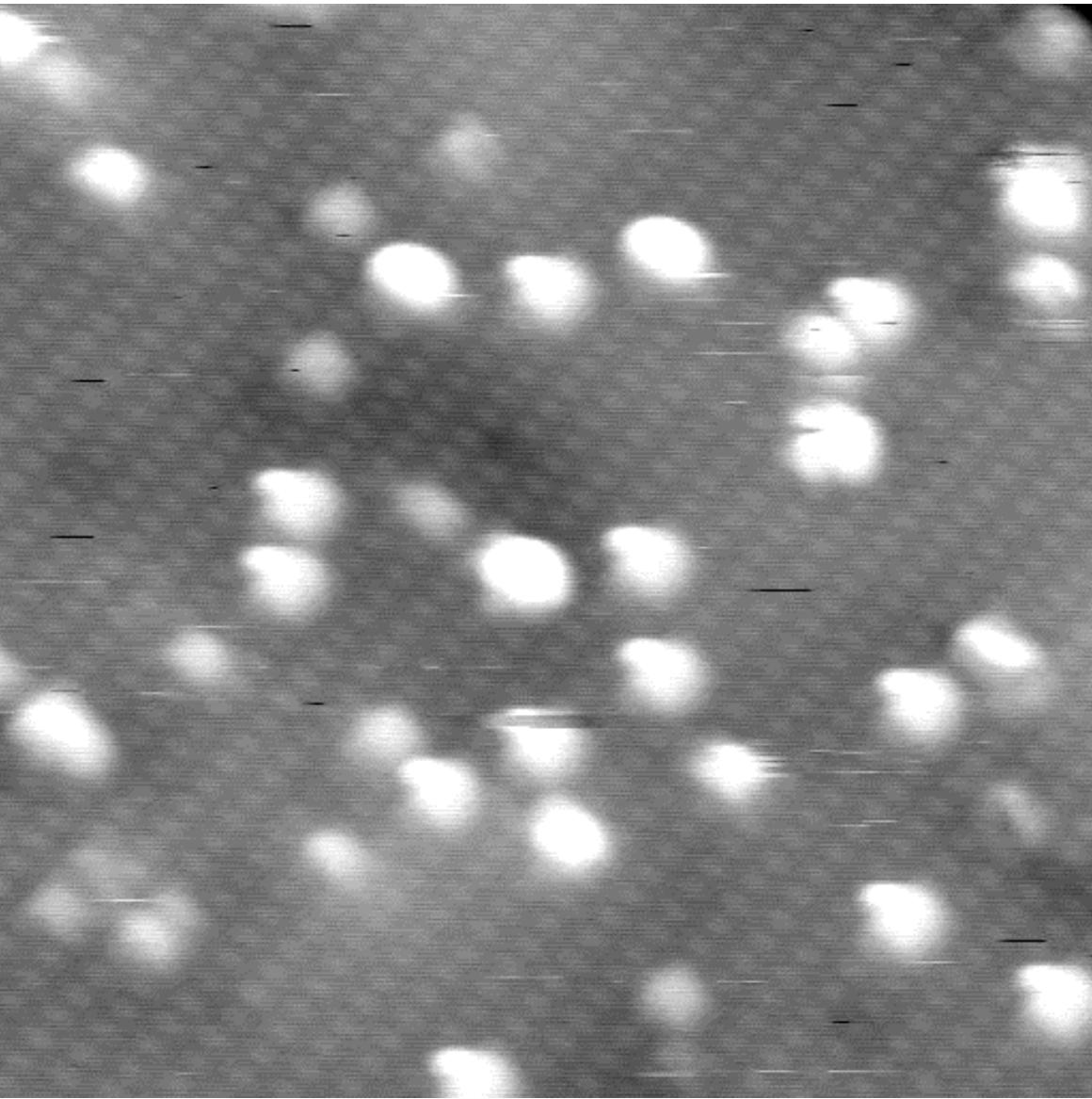
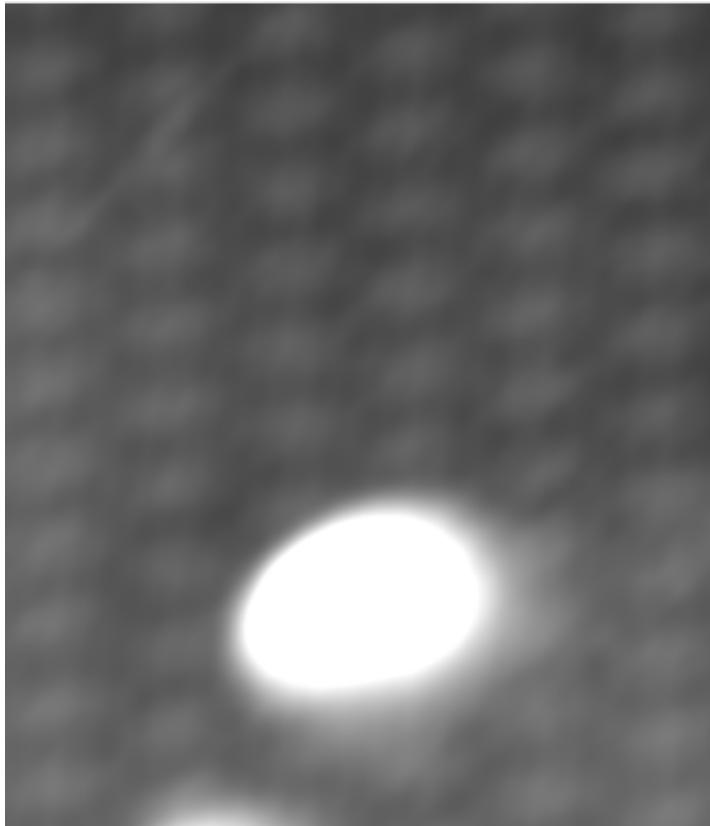


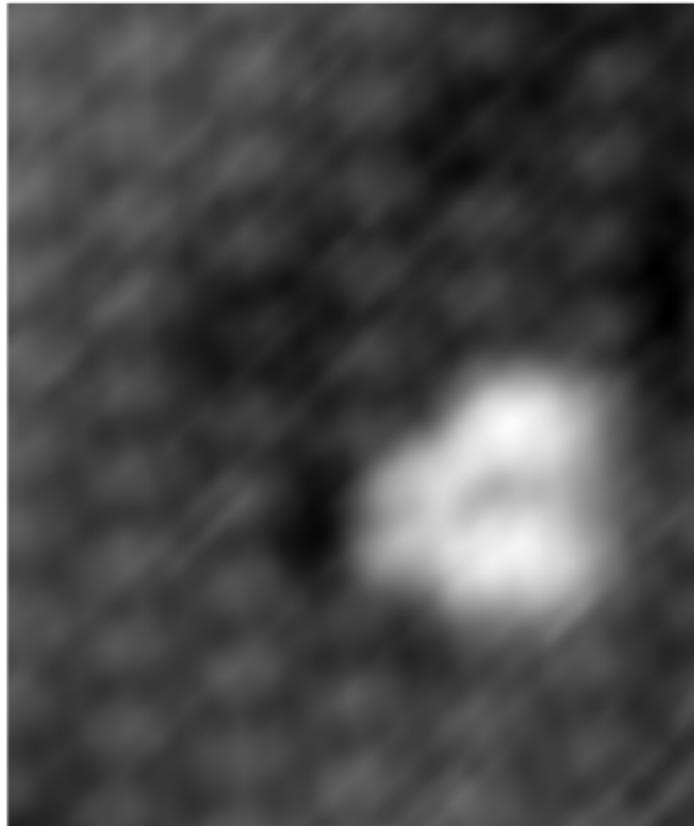
Vanadium figures



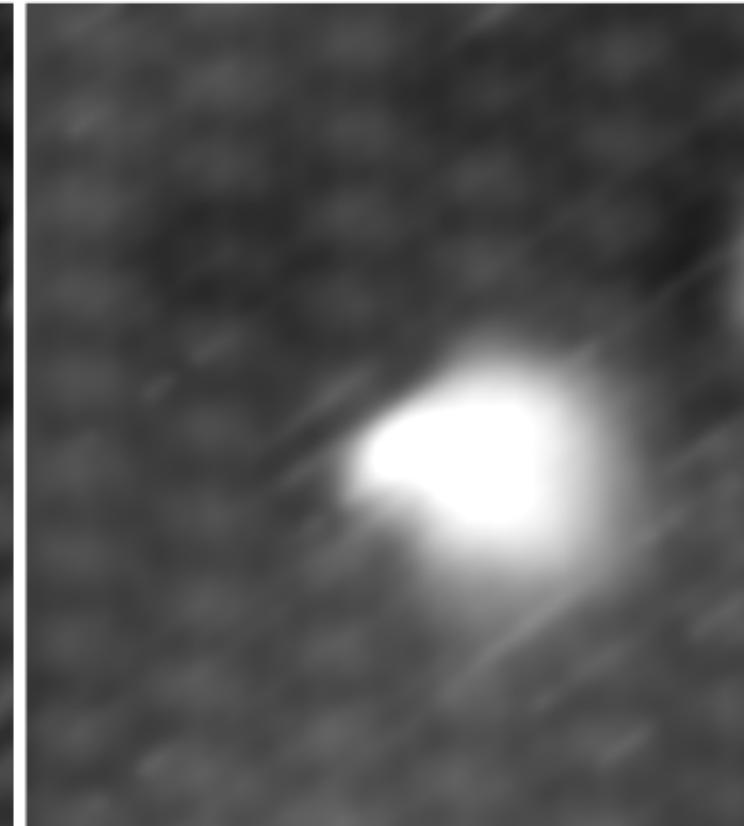
As-Deposited



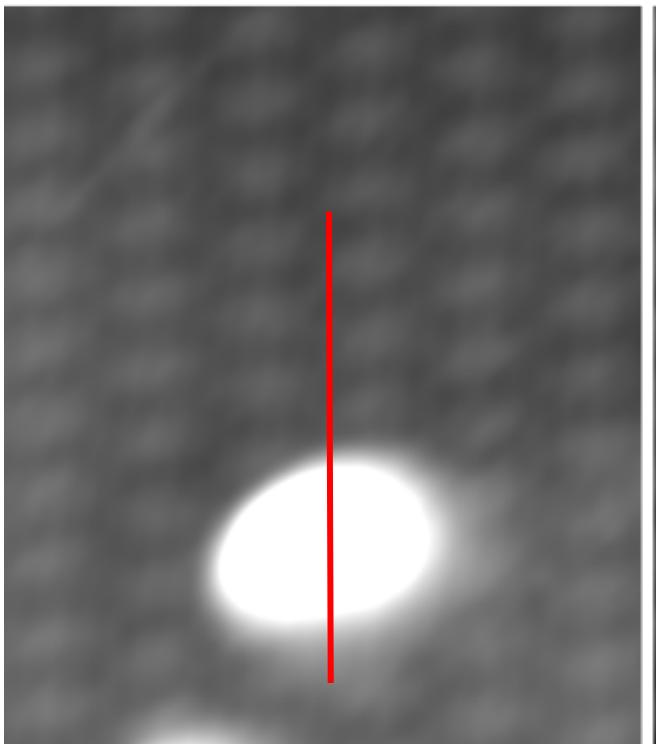
During Water exposure



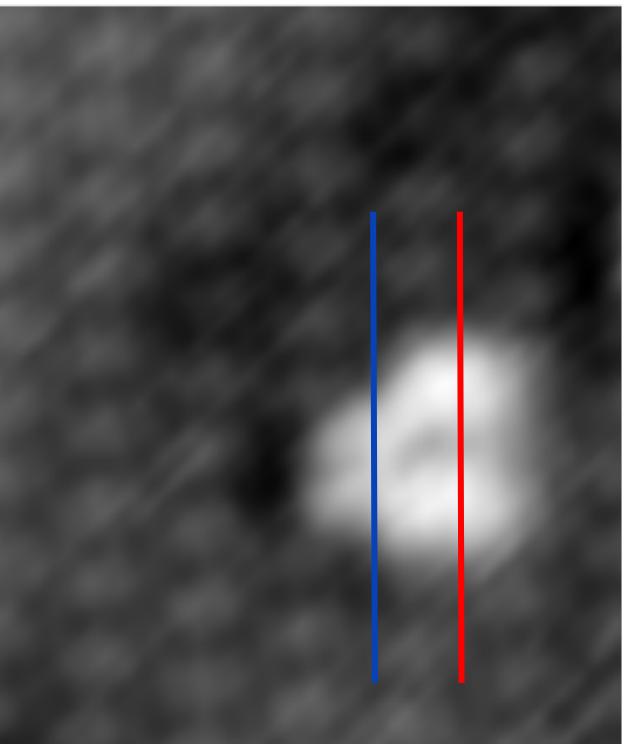
After Water Exposure



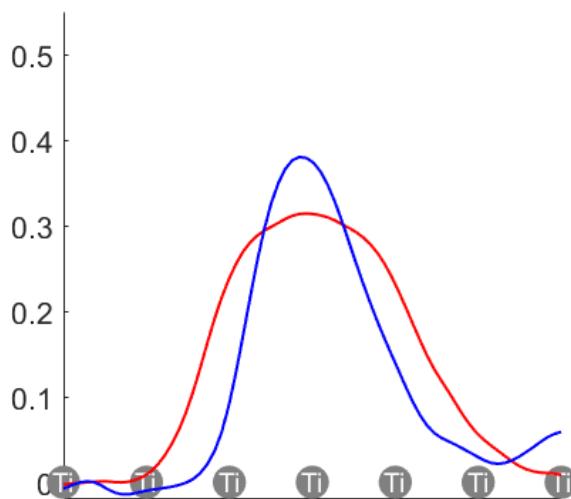
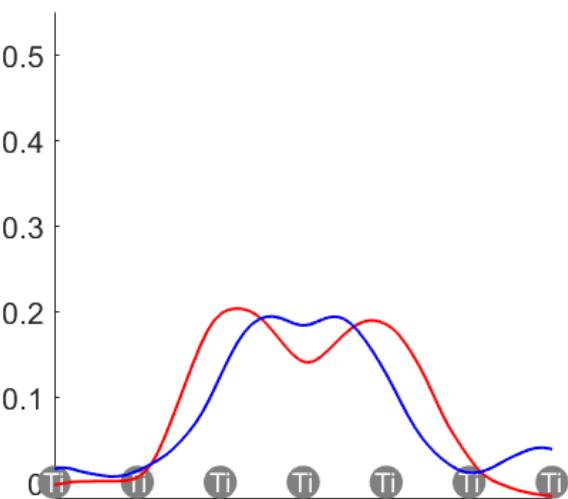
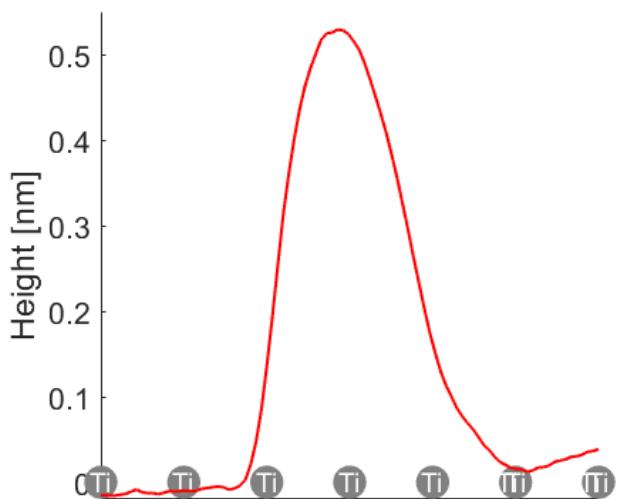
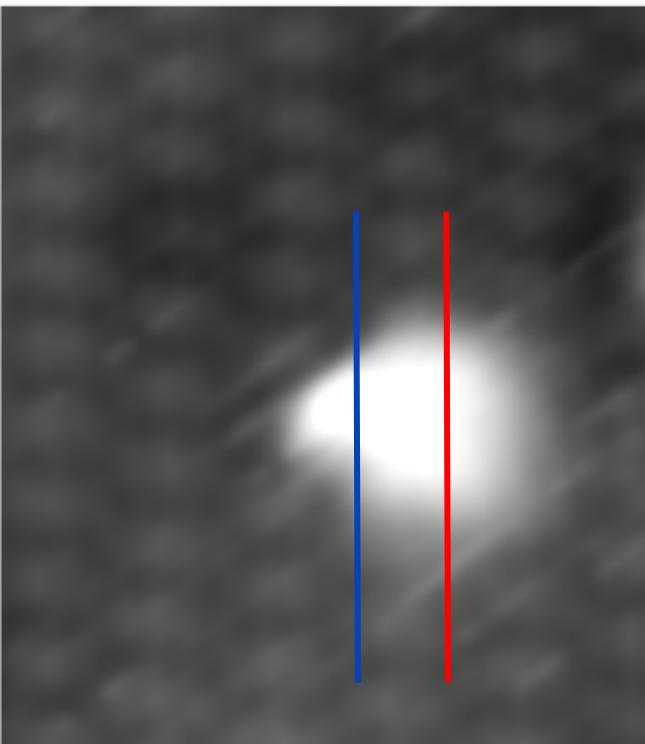
As-Deposited



During Water exposure



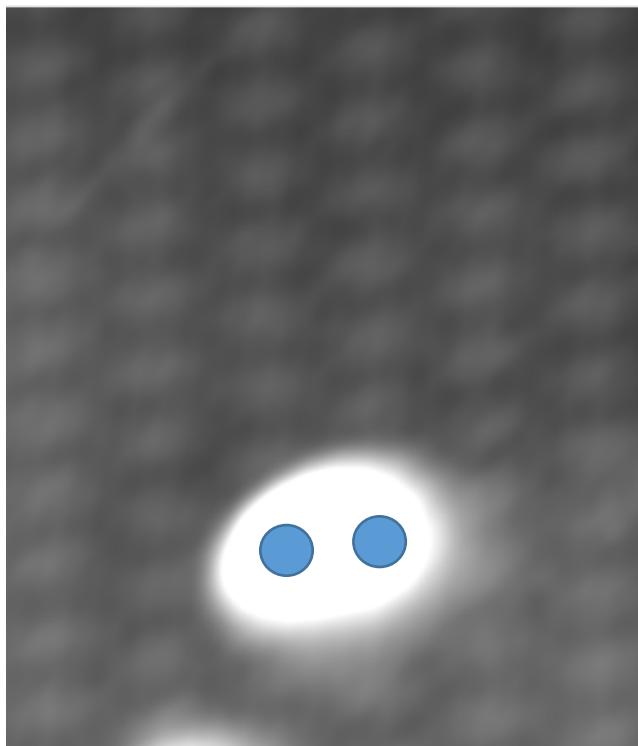
After Water Exposure



model suggestions

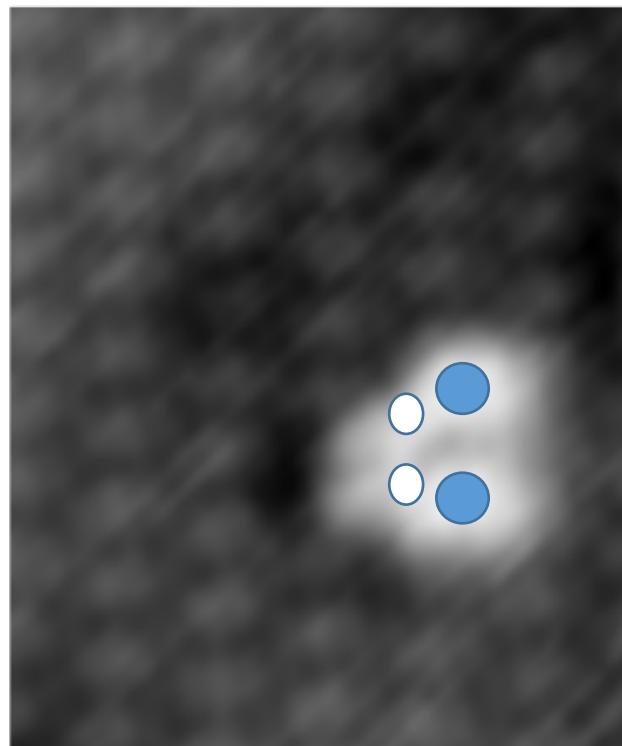
● = V

As-Deposited



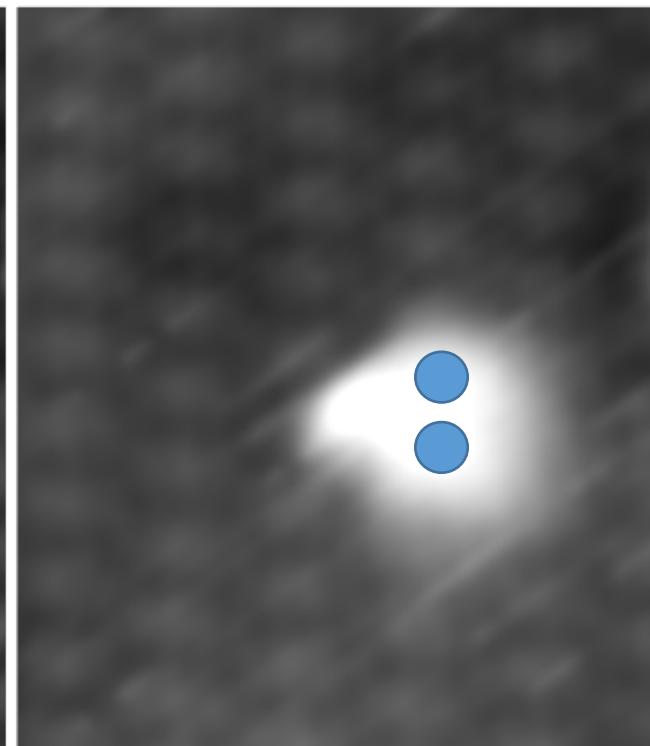
V2O5

During Water exposure



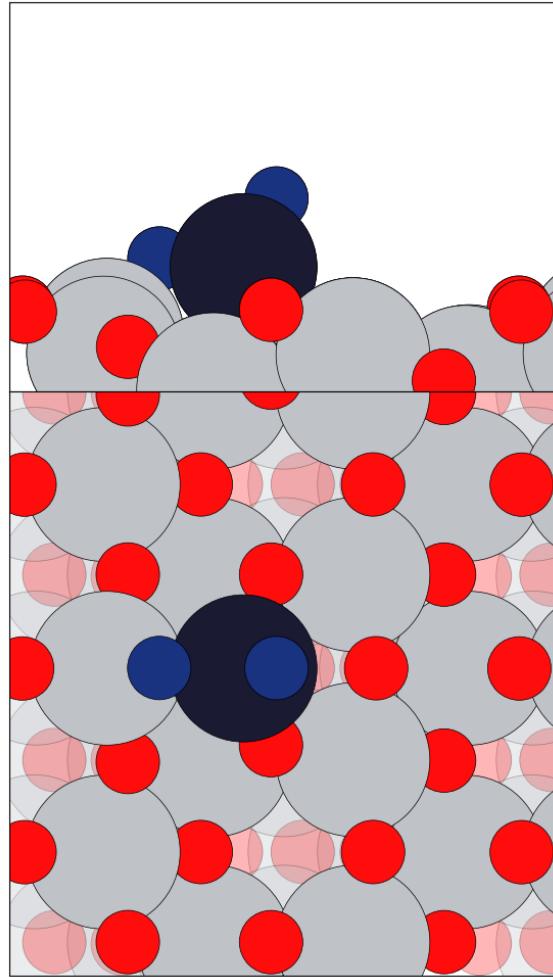
2 X VO₃H

After Water Exposure



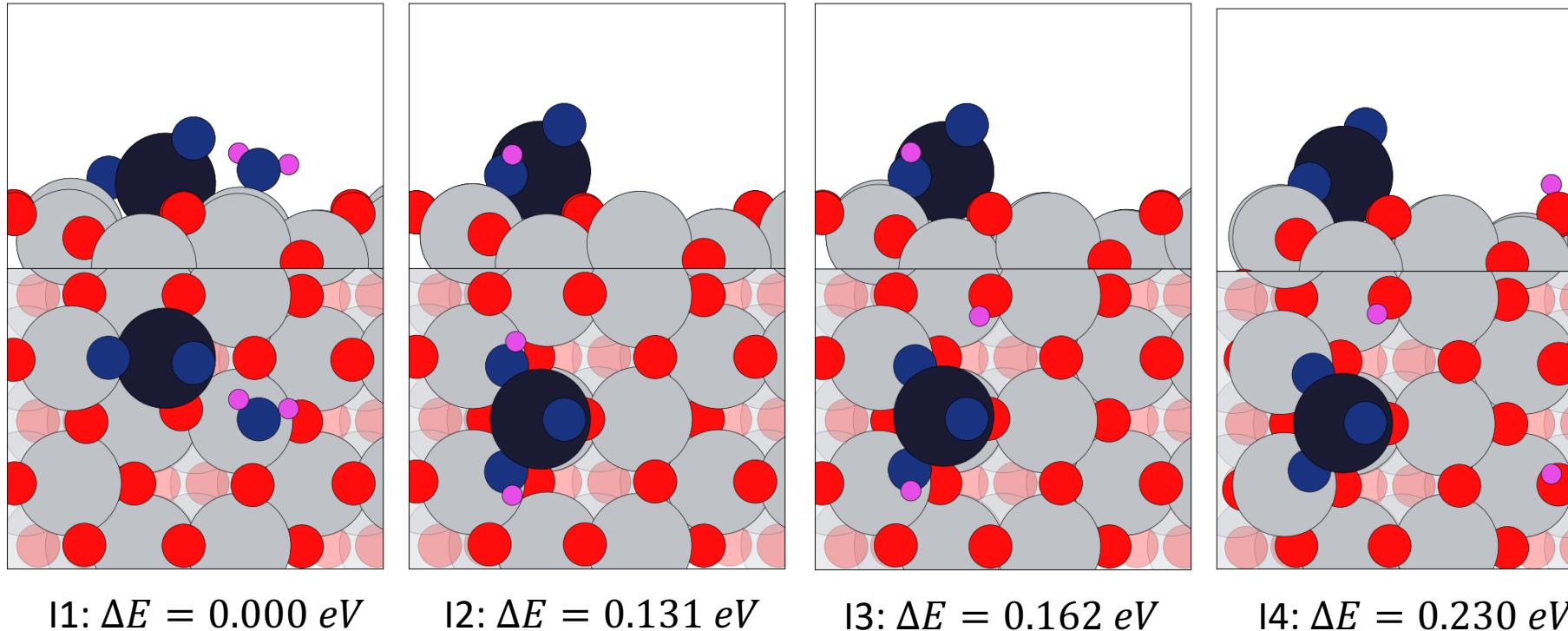
V2O5

VO₂ Clusters with O_v (1by2 Super cell)

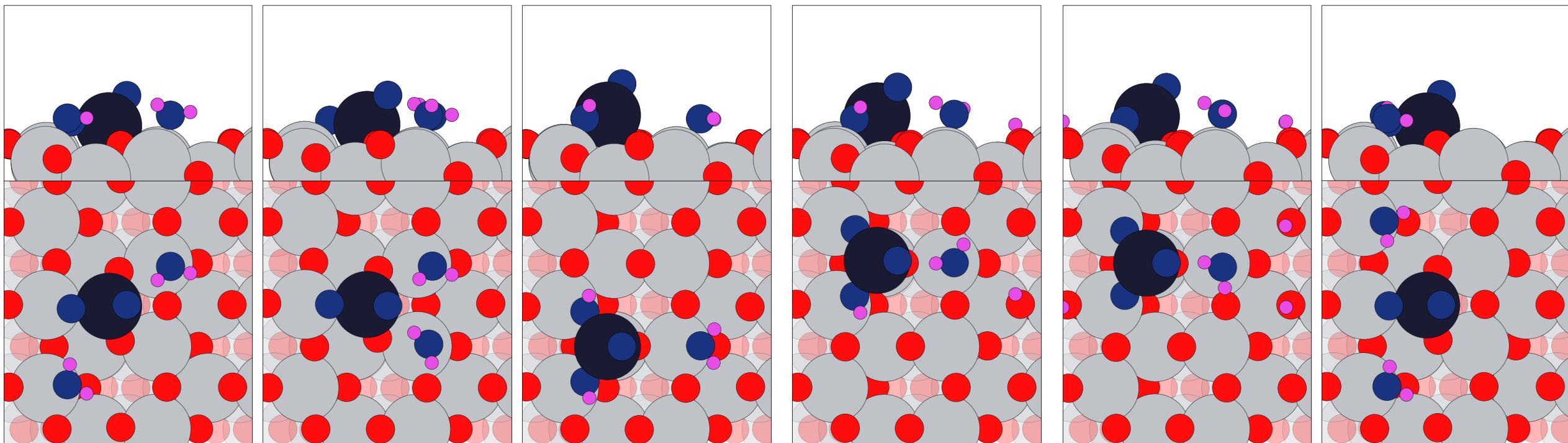


|1: $\Delta E = 0.000 \text{ eV}$

$\text{VO}_2 + \text{H}_2\text{O}$ Clusters with O_v (1by2 Super cell)



$\text{VO}_2 + 2\text{H}_2\text{O}$ Clusters with O_v (1by3 Super cell)



I1: $\Delta E = 0.000 \text{ eV}$

I2: $\Delta E = 0.021 \text{ eV}$

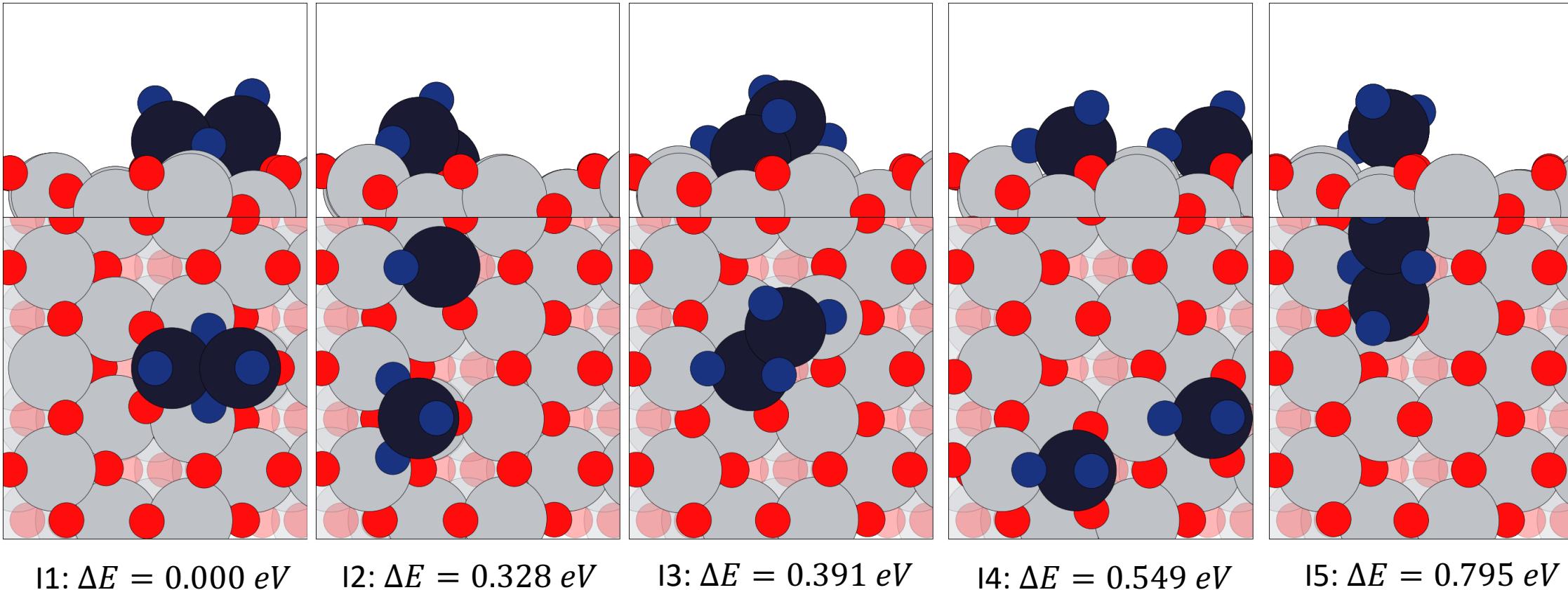
I3: $\Delta E = 0.053 \text{ eV}$

I4: $\Delta E = 0.071 \text{ eV}$

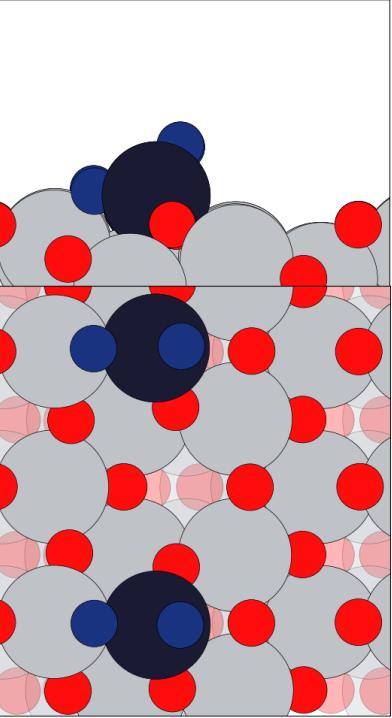
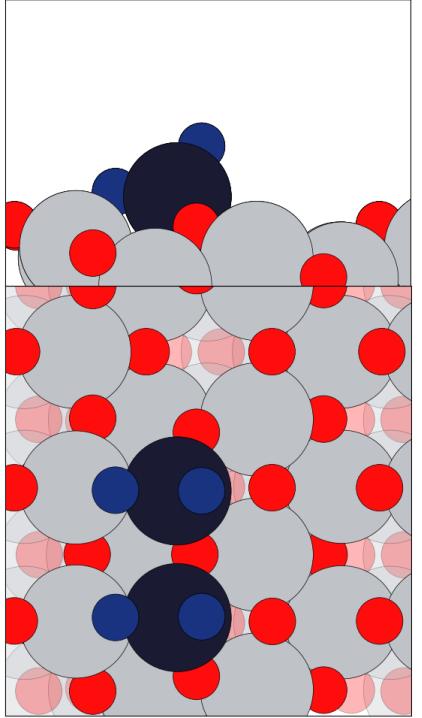
I5: $\Delta E = 0.176 \text{ eV}$

I6: $\Delta E = 0.208 \text{ eV}$

V_2O_4 Clusters with O_v (1by3 Super cell)



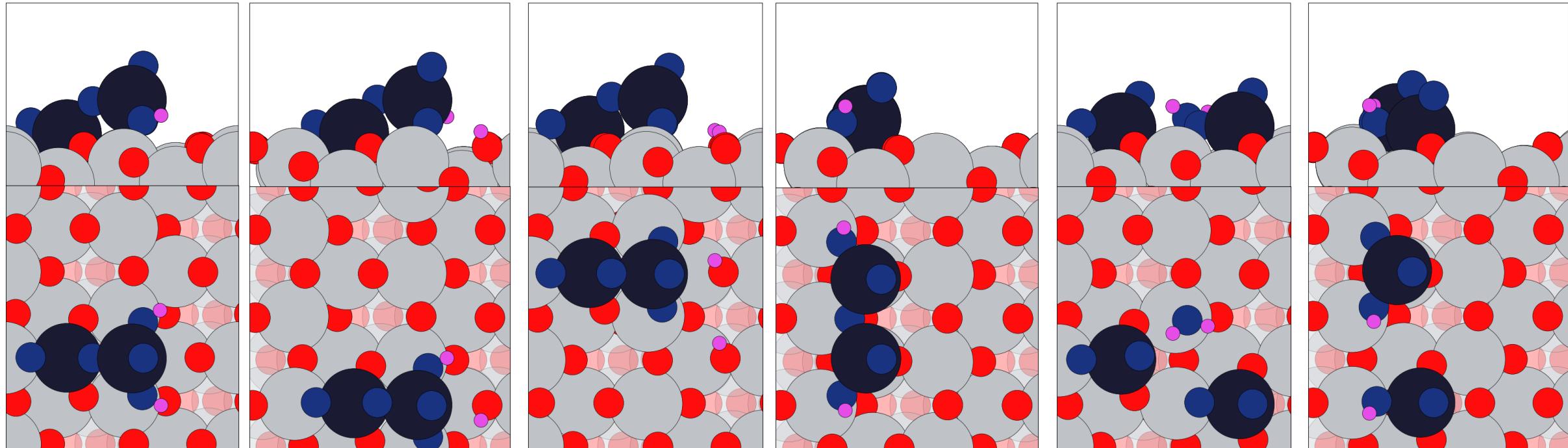
V_2O_4 Clusters with O_v (1by3 Super cell)



I6: $\Delta E = 1.100 \text{ eV}$

I7: $\Delta E = 1.194 \text{ eV}$

$\text{V}_2\text{O}_4 + \text{H}_2\text{O}$ Clusters with O_v (1by3 Super cell)



I1: $\Delta E = 0.000 \text{ eV}$

I2: $\Delta E = 0.417 \text{ eV}$

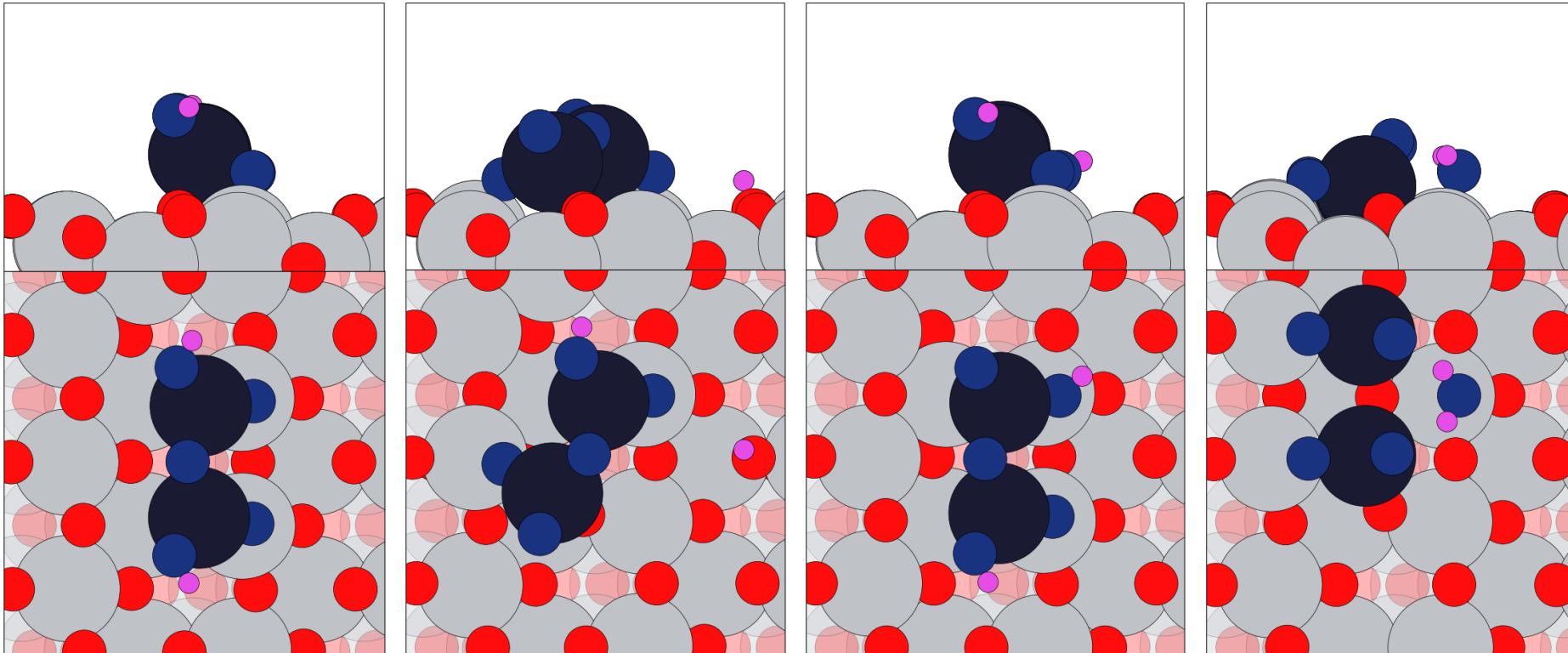
I3: $\Delta E = 0.468 \text{ eV}$

I4: $\Delta E = 0.600 \text{ eV}$

I5: $\Delta E = 0.664 \text{ eV}$

I6: $\Delta E = 0.703 \text{ eV}$

$\text{V}_2\text{O}_4 + \text{H}_2\text{O}$ Clusters with O_v (1by3 Super cell)



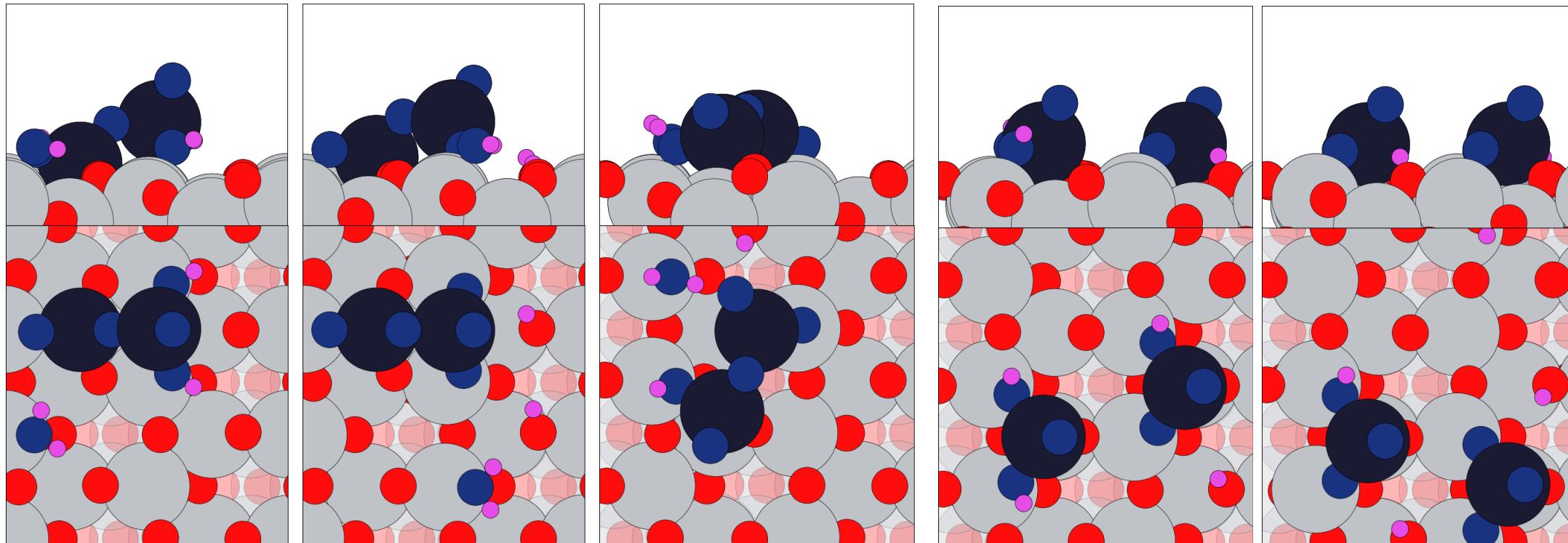
I7: $\Delta E = 0.837 \text{ eV}$

I8: $\Delta E = 0.931 \text{ eV}$

I9: $\Delta E = 0.982 \text{ eV}$

I10: $\Delta E = 1.180 \text{ eV}$

$\text{V}_2\text{O}_4 + 2\text{H}_2\text{O}$ Clusters with O_v (1by3 Super cell)



I1: $\Delta E = 0.000 \text{ eV}$

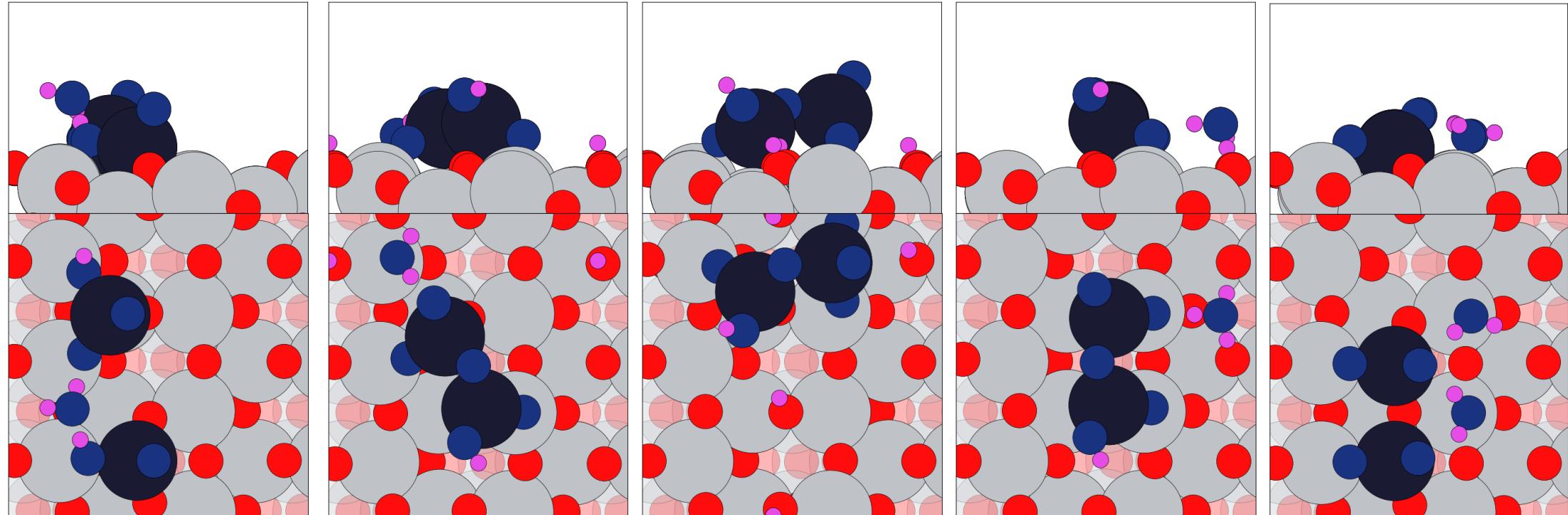
I2: $\Delta E = 0.409 \text{ eV}$

I3: $\Delta E = 0.541 \text{ eV}$

I4: $\Delta E = 0.574 \text{ eV}$

I5: $\Delta E = 0.633 \text{ eV}$

$\text{V}_2\text{O}_4 + 2\text{H}_2\text{O}$ Clusters with O_v (1by3 Super cell)



I6: $\Delta E = 0.803 \text{ eV}$

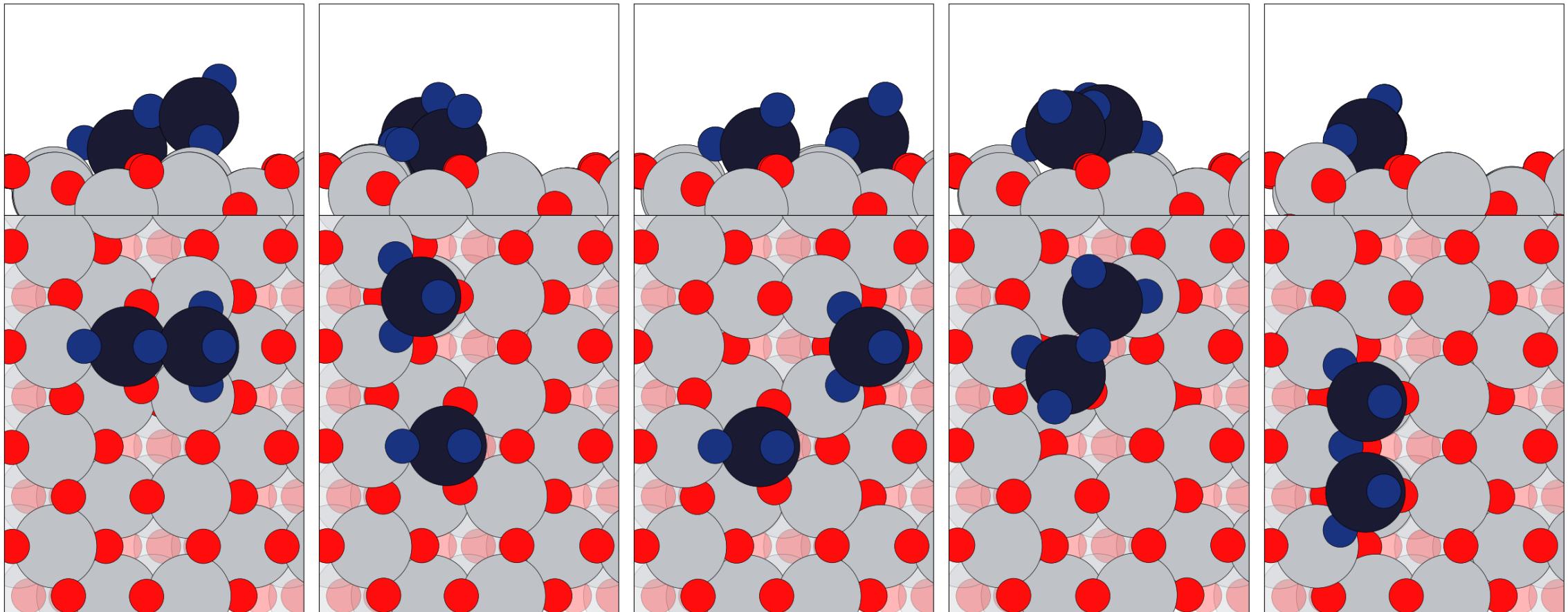
I7: $\Delta E = 0.837 \text{ eV}$

I8: $\Delta E = 0.874 \text{ eV}$

I9: $\Delta E = 0.989 \text{ eV}$

I10: $\Delta E = 1.059 \text{ eV}$

V_2O_5 Clusters with O_v (1by4 Super cell)



I1: $\Delta E = 0.000 \text{ eV}$

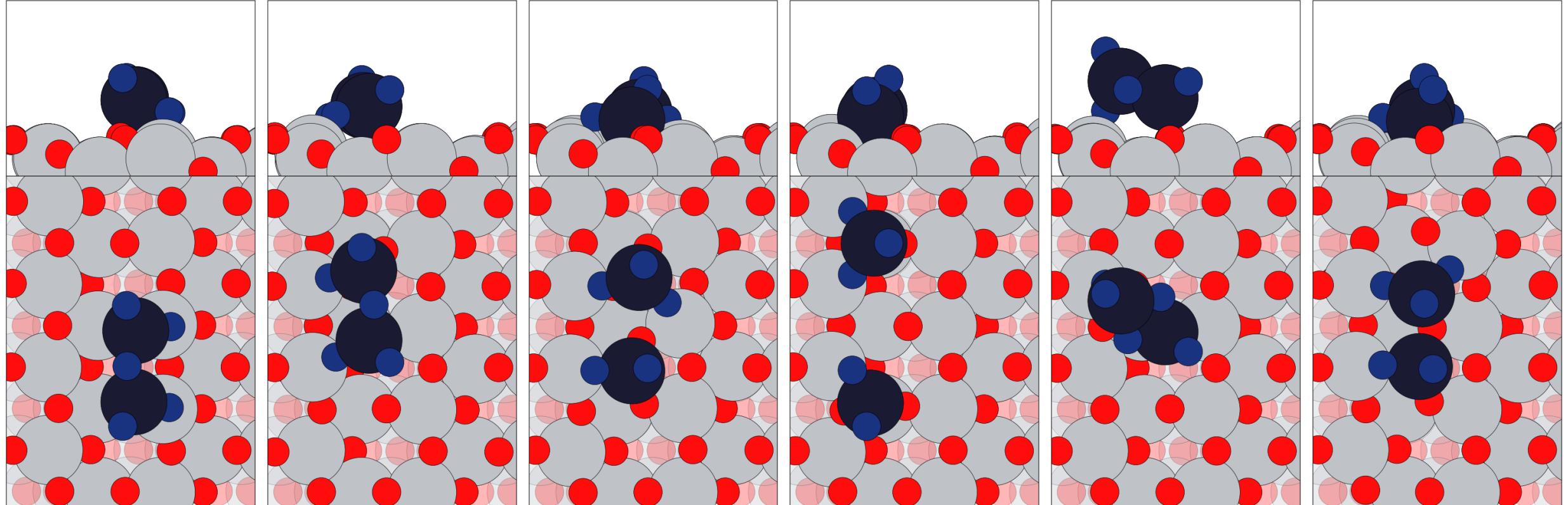
I2: $\Delta E = 0.127 \text{ eV}$

I3: $\Delta E = 0.131 \text{ eV}$

I4: $\Delta E = 0.257 \text{ eV}$

I5: $\Delta E = 0.326 \text{ eV}$

V_2O_5 Clusters with O_v (1by4 Super cell)



I6: $\Delta E = 0.420 \text{ eV}$

I7: $\Delta E = 0.814 \text{ eV}$

I8: $\Delta E = 1.065 \text{ eV}$

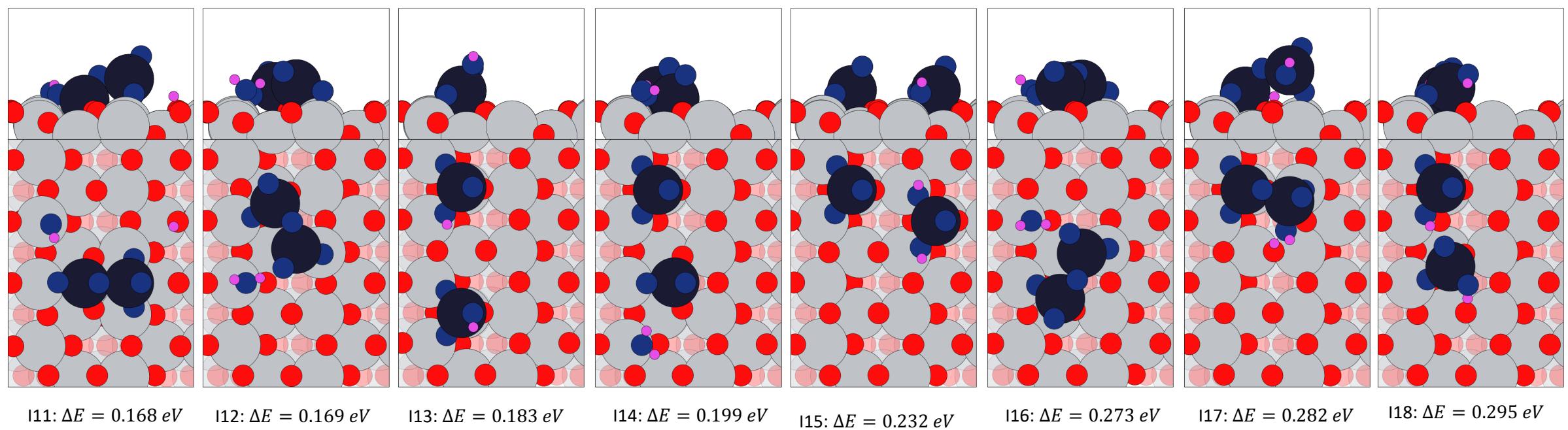
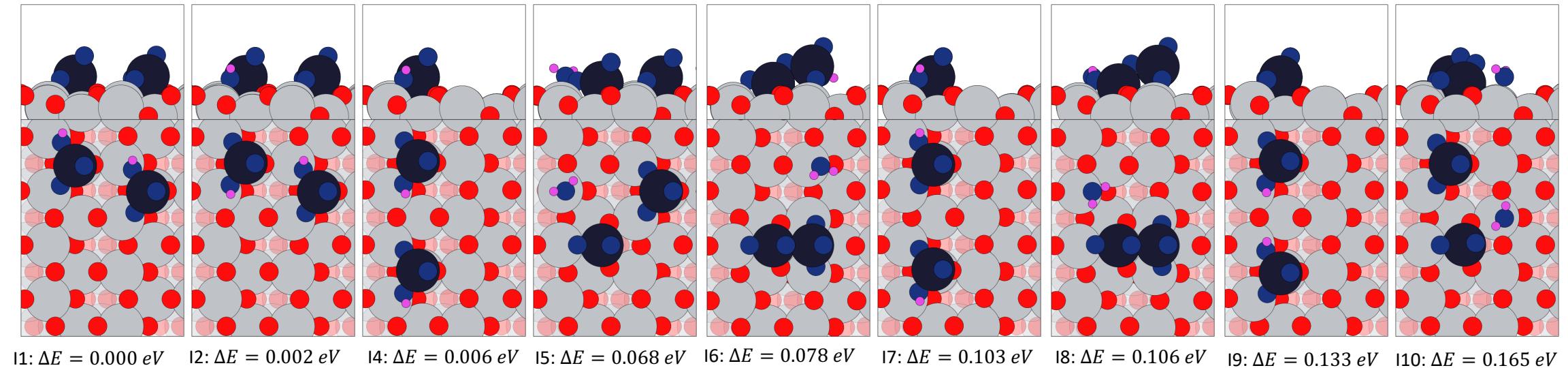
I9: $\Delta E = 1.164 \text{ eV}$

I10: $\Delta E = 1.244 \text{ eV}$

I11: $\Delta E = 2.238 \text{ eV}$

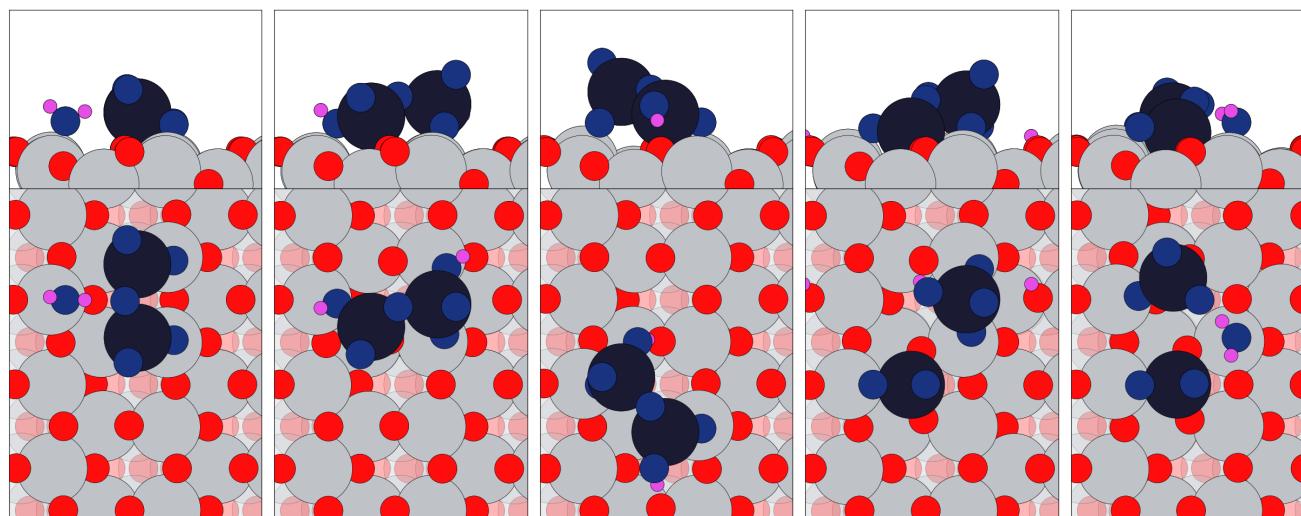
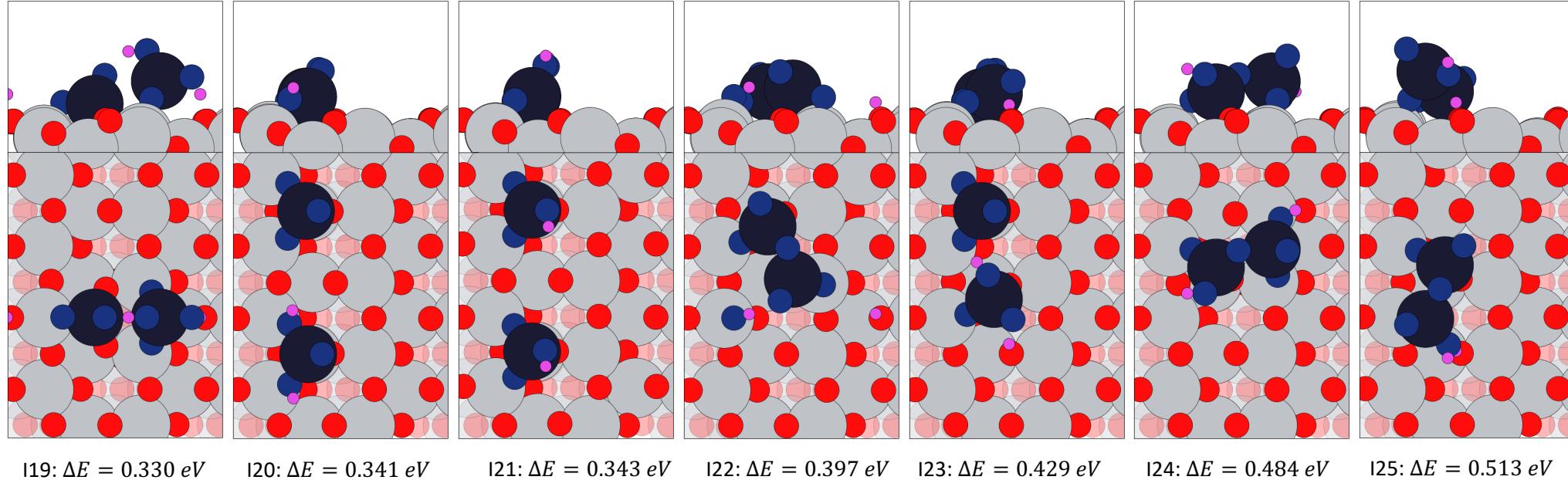
V_2O_5 Clusters with O_v (1by4 cell)

$V_2O_5 + H_2O \xrightarrow{TiO_2 \text{ (101) surface } O \text{ vacancy}}$



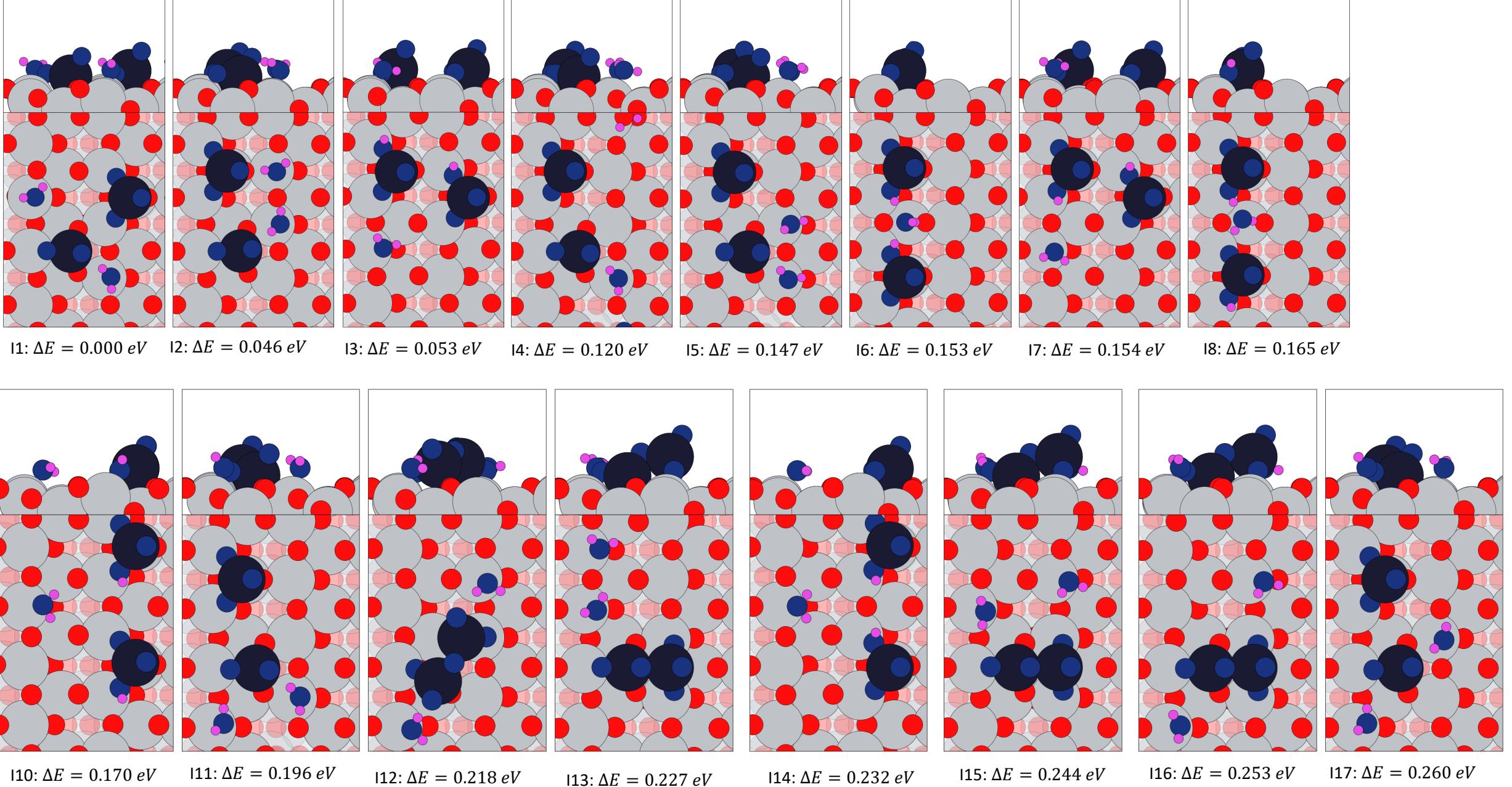
V_2O_5 Clusters with O_v (1by4 cell)

$V_2O_5 + H_2O \xrightarrow{TiO_2(101) \text{ surface } O \text{ vacancy}}$



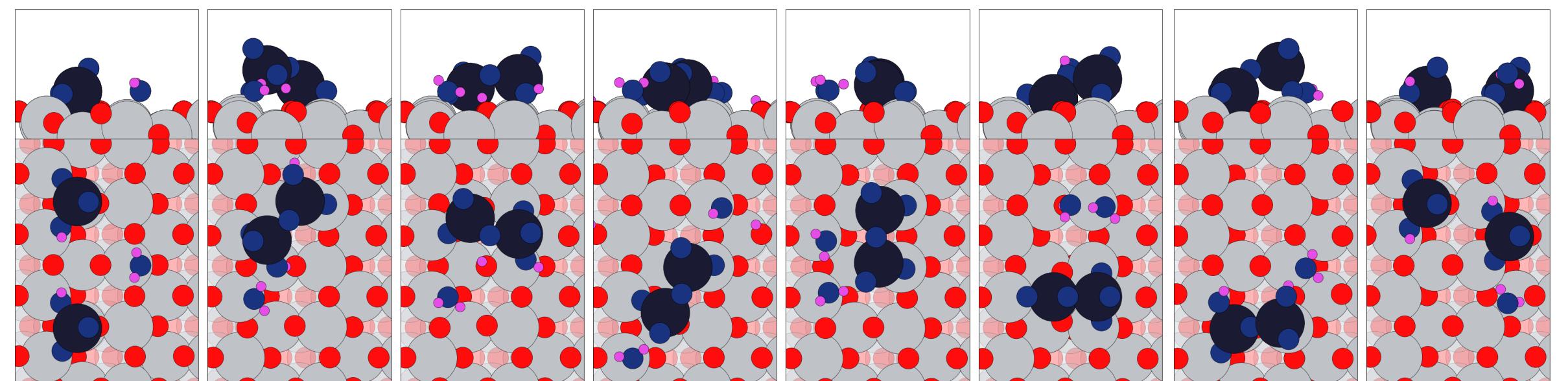
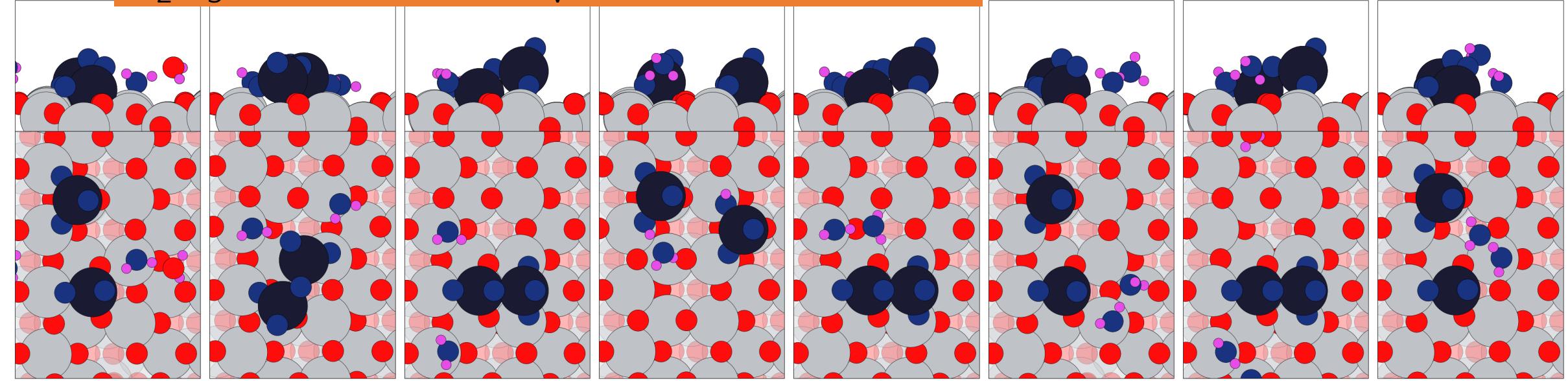
V_2O_5 Clusters with O_v (1by4 Super cell)

$V_2O_5 + 2 H_2O \xrightarrow{TiO_2(101) \text{ surface } O \text{ vacancy}}$



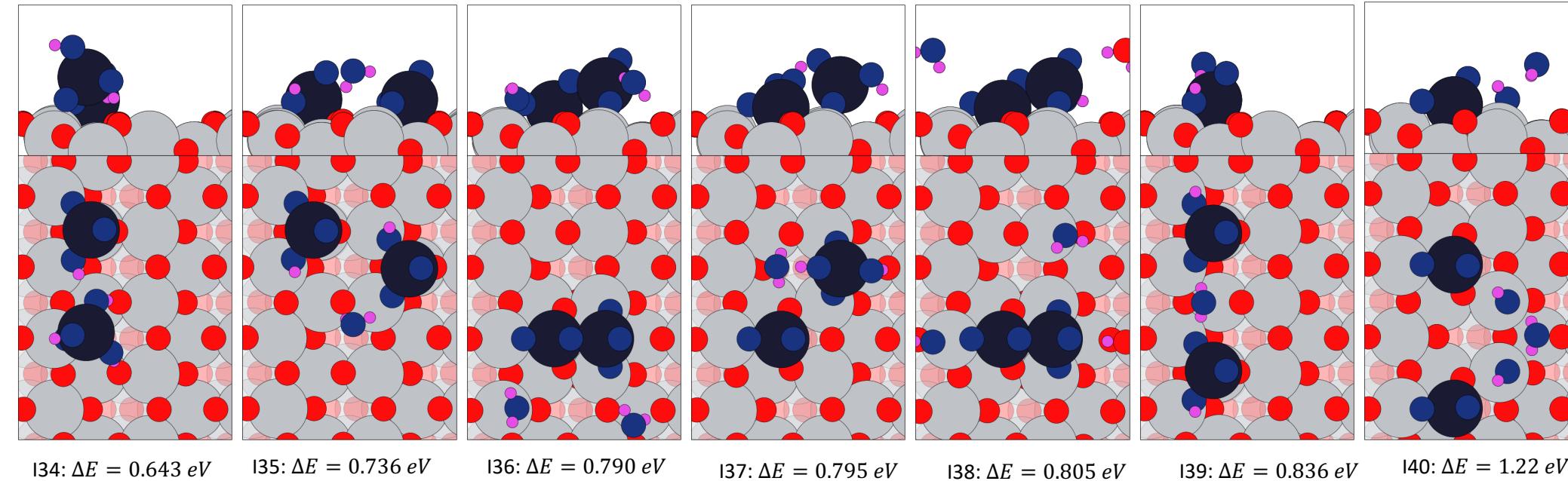
V_2O_5 Clusters with O_v (1by4 Super cell)

$V_2O_5 + 2 H_2O \xrightarrow{TiO_2(101) \text{ surface } O \text{ vacancy}}$

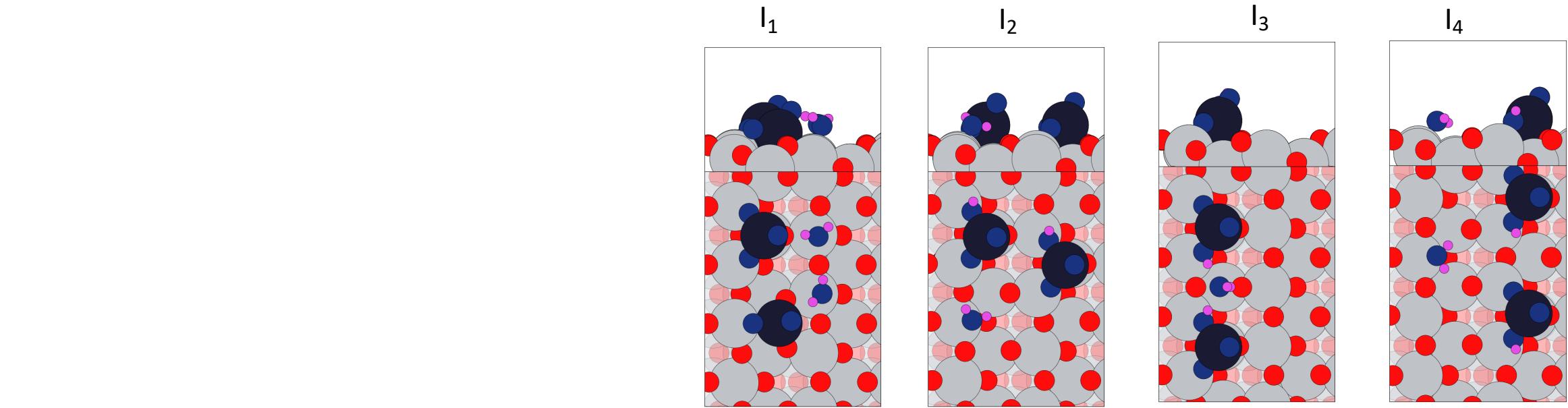


V_2O_5 Clusters with O_v (1by4 Super cell)

$V_2O_5 + 2 H_2O \xrightarrow{TiO_2(101) \text{ surface } O \text{ vacancy}}$



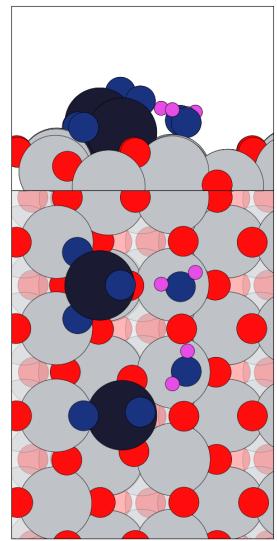
Method Vs Energy Order



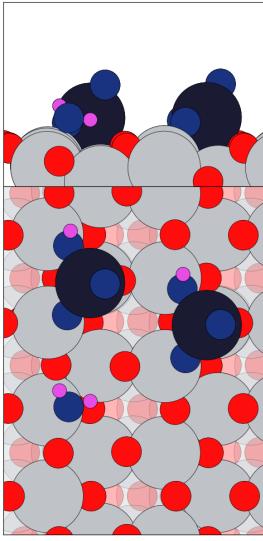
Method ($f_{\text{cut}}=0.023 \text{ eV/Ang}$)	$I_1/\Delta E(\text{eV}) (O_v)$	$I_2/\Delta E(\text{eV})(O_v)$	$I_3/\Delta E(\text{eV})(O_v)$	$I_4/\Delta E(\text{eV})(O_v)$
GPAW (PW(500 eV),PBE,dzp,(2,2,1))	0.00	-0.476	-0.103	-0.411
GPAW (PW(500 eV),PBE,dzp,(2,2,1), U(4.0))	0.000	0.006	0.106	0.124
GPAW (PW(500 eV),PBE,dzp,(4,4,1), U(4.0))	0.000	0.006	0.106	0.123
CP2K (GPW(400 Ry),PBE,dzvp)	0.000	-1.154	-0.745	-0.951
CP2K (GPW(400 Ry),PBE,dispersion (dftd3),dzvp)	0.000	-1.017	-0.584	-0.719

Method Vs Energy Order

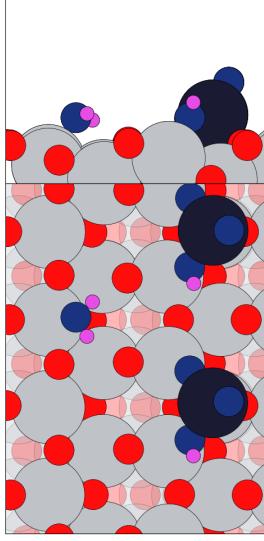
$M_1 = \text{CP2K} (\text{GPW}(400 \text{ Ry}), \text{PBE}, \text{dzvp})$ $M_2 = \text{GPAW} (\text{PW}(500 \text{ eV}), \text{PBE}, \text{dzp}, (2,2,1))$ $M_3 = \text{GPAW} (\text{PW}(500 \text{ eV}), \text{PBE}, \text{dzp}, (2,2,1), \text{U}(4.0))$



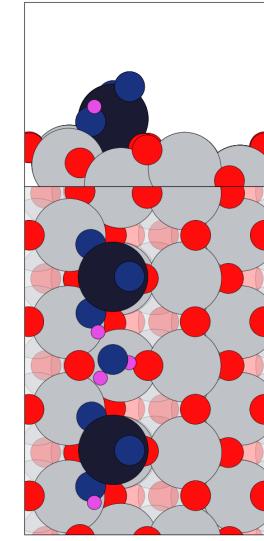
$M_1 : \Delta E = 0.000 \text{ eV}$



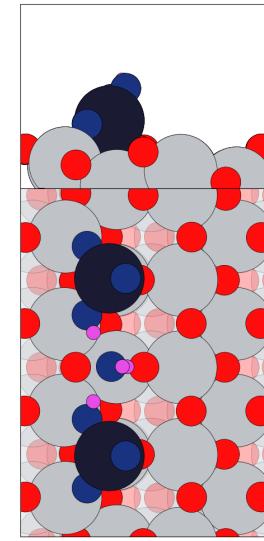
$M_1 : \Delta E = -1.154 \text{ eV}$



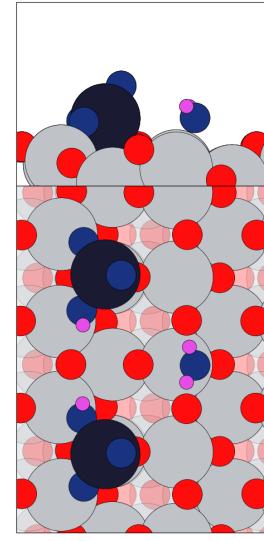
$M_1 : \Delta E = -0.951 \text{ eV}$



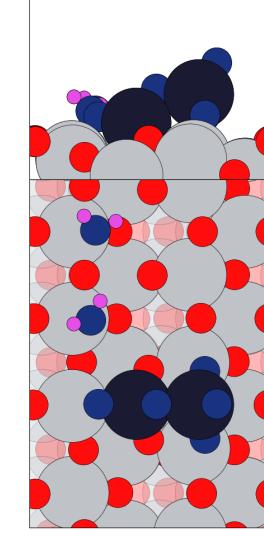
$M_1 : \Delta E = -0.764 \text{ eV}$



$M_1 : \Delta E = -0.745 \text{ eV}$



$M_1 : \Delta E = -0.742 \text{ eV}$



$M_1 : \Delta E = 0.159 \text{ eV}$

$M_2 : \Delta E = 0.000 \text{ eV}$

$M_2 : \Delta E = -0.405 \text{ eV}$

$M_2 : \Delta E = -0.302 \text{ eV}$

$M_2 : \Delta E = 0.061 \text{ eV}$

$M_2 : \Delta E = 0.102 \text{ eV}$

$M_2 : \Delta E = 0.095 \text{ eV}$

$M_2 : \Delta E = -0.230 \text{ eV}$

$M_3 : \Delta E = 0.000 \text{ eV}$

$M_3 : \Delta E = 0.006 \text{ eV}$

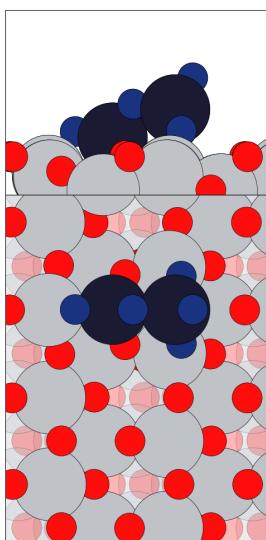
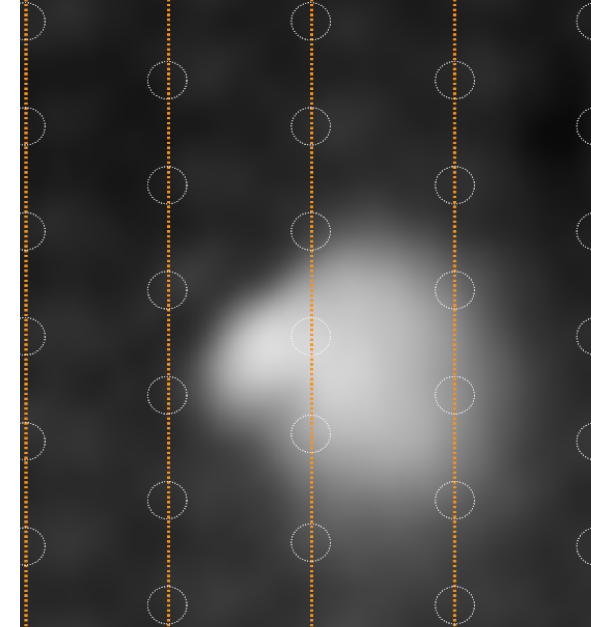
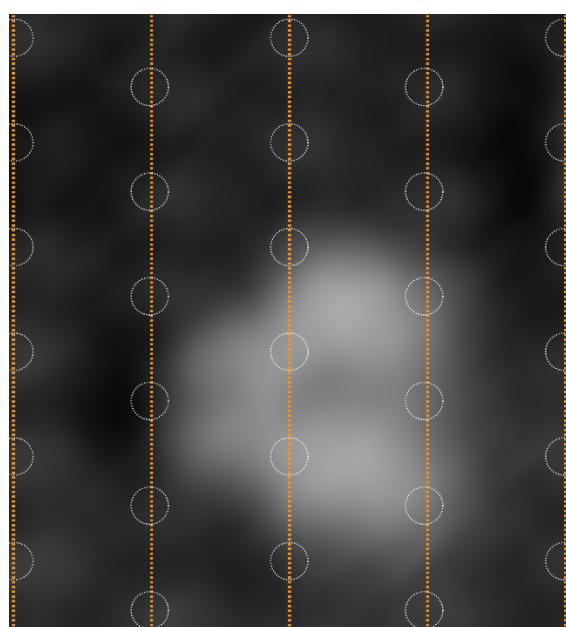
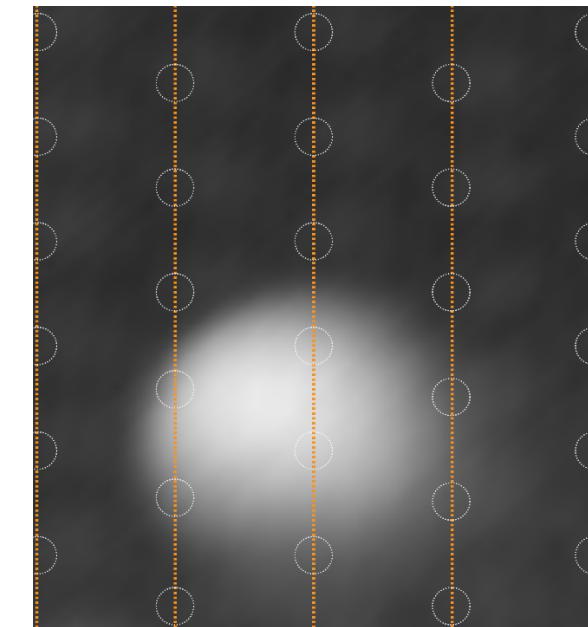
$M_3 : \Delta E = 0.124 \text{ eV}$

$M_3 : \Delta E = 0.119 \text{ eV}$

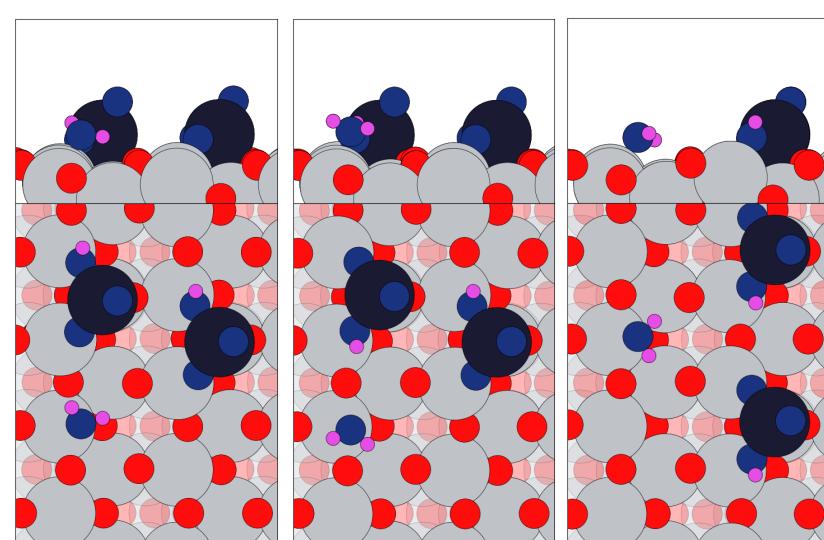
$M_3 : \Delta E = 0.106 \text{ eV}$

$M_3 : \Delta E = 0.379 \text{ eV}$

$M_3 : \Delta E = 0.180 \text{ eV}$



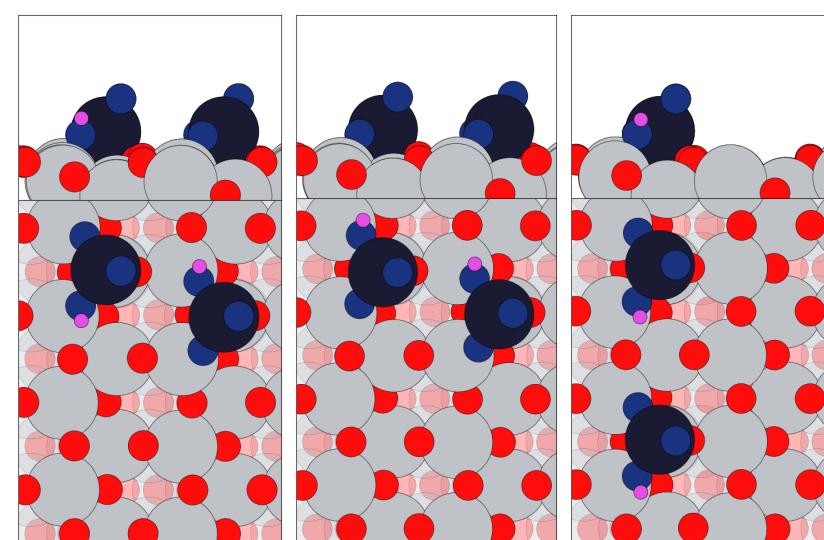
$\Delta E = 0.000 \text{ eV}$



$\Delta E = 0.000 \text{ eV}$

$\Delta E = 0.031 \text{ eV}$

$\Delta E = 0.100 \text{ eV}$

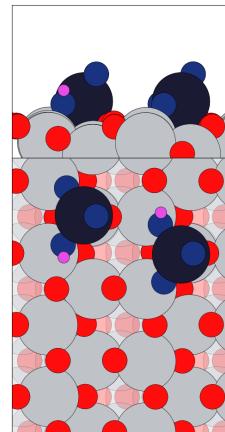
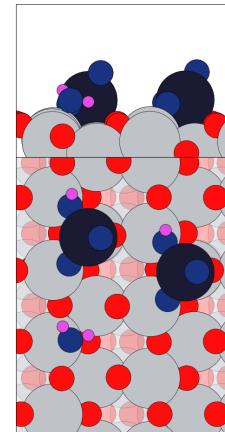
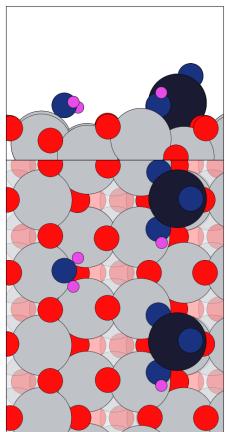
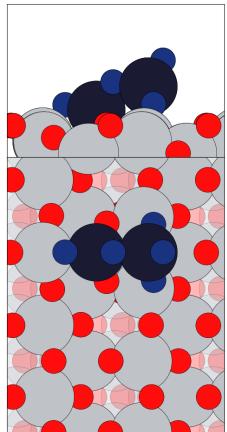
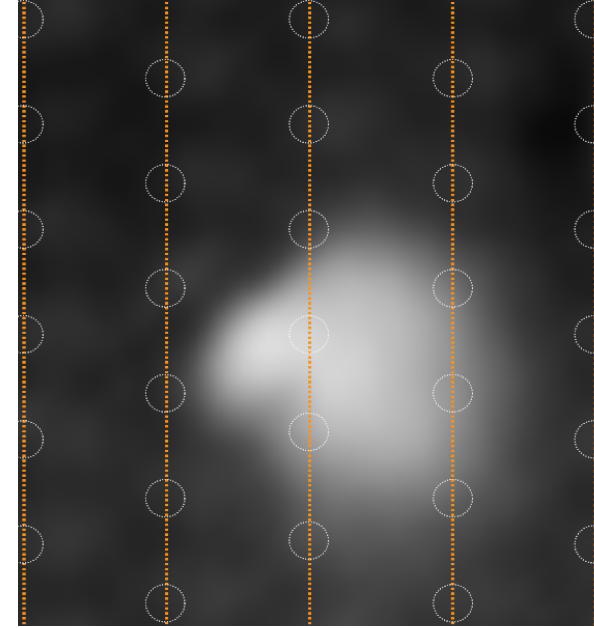
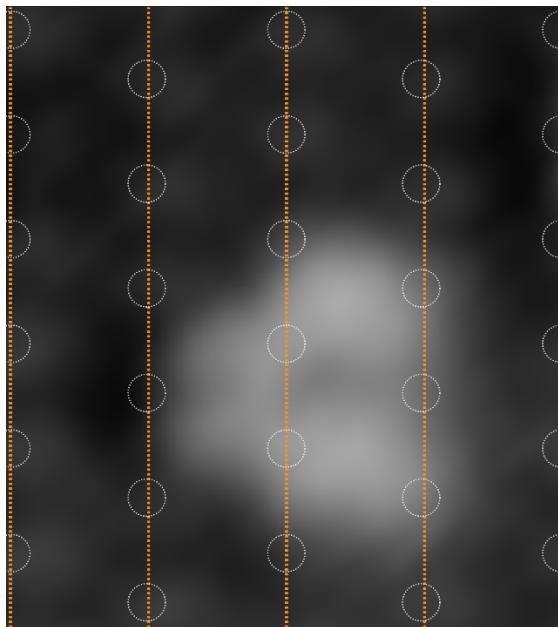
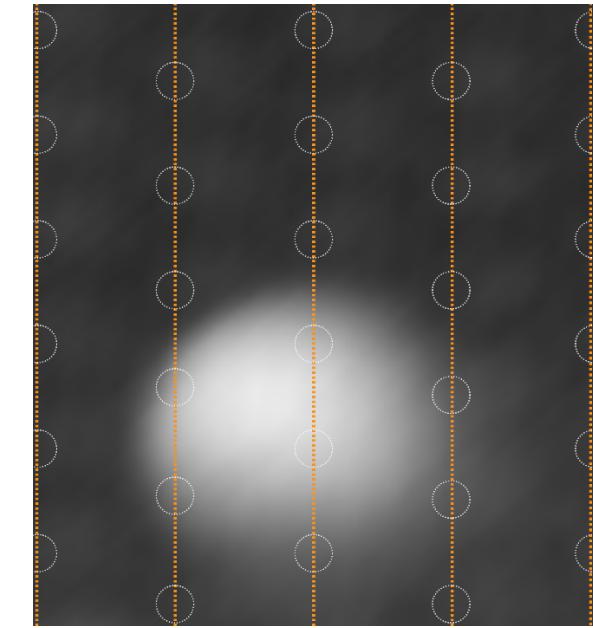


$\Delta E = 0.000 \text{ eV}$

$\Delta E = 0.05 \text{ eV}$

$\Delta E = 0.08 \text{ eV}$

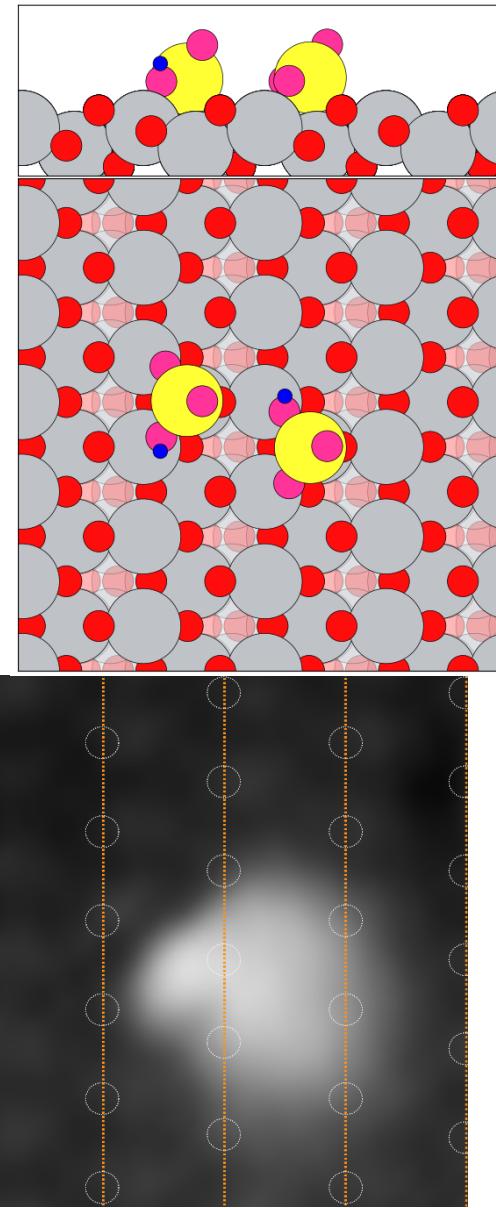
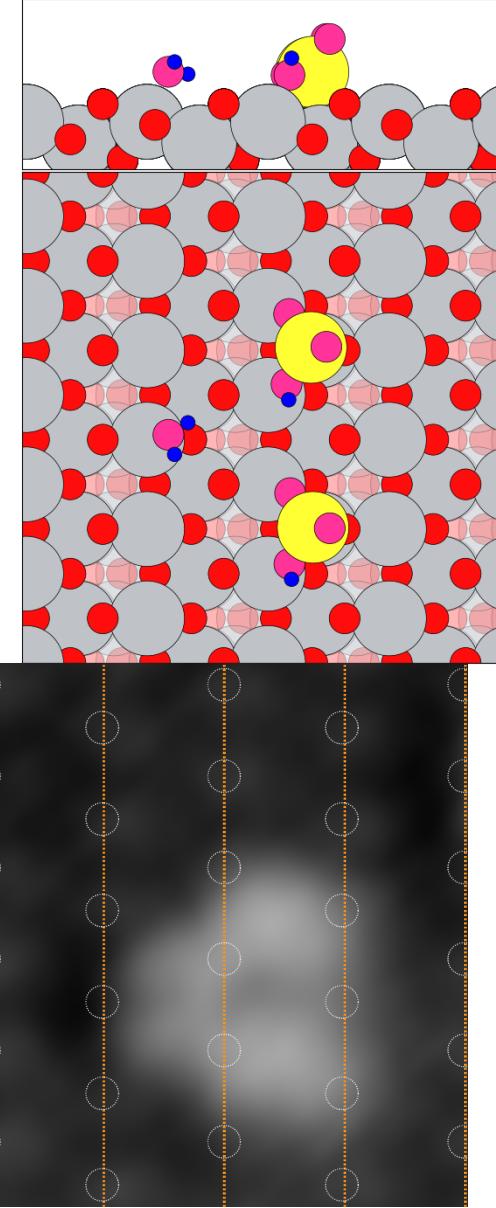
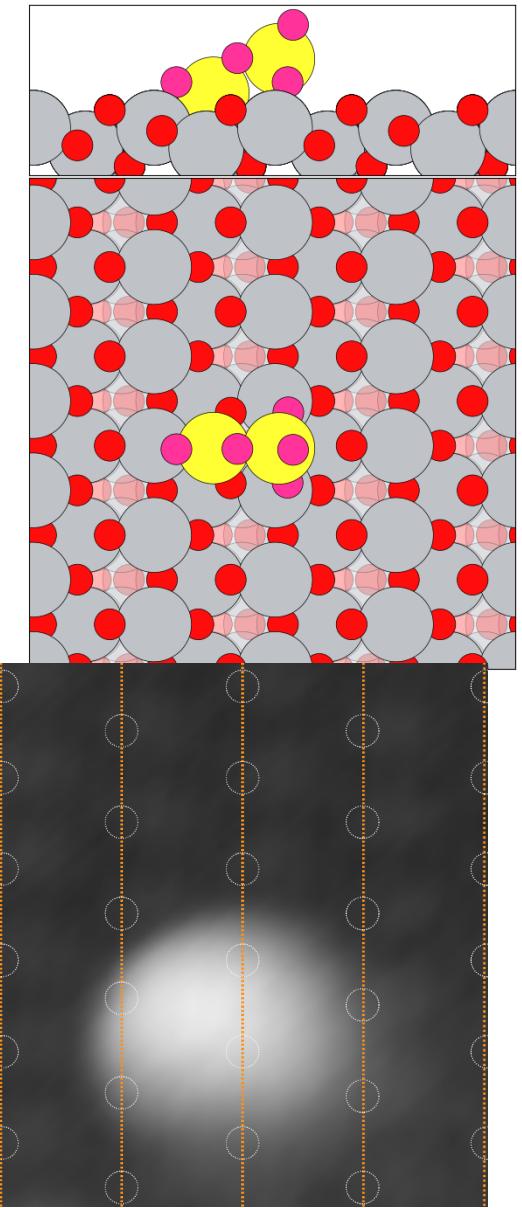
All the structures optimized with 1×4 super cell



$$P_{298\text{ K}} = 51\% \quad P_{298\text{ K}} = 49\%$$

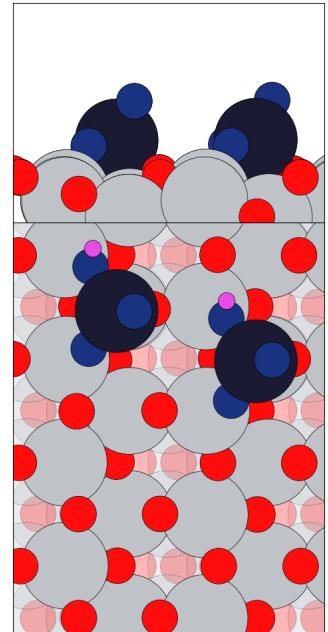
Calculations done in 2×6 super cell only for two structures during exposure.

Figures for Paper

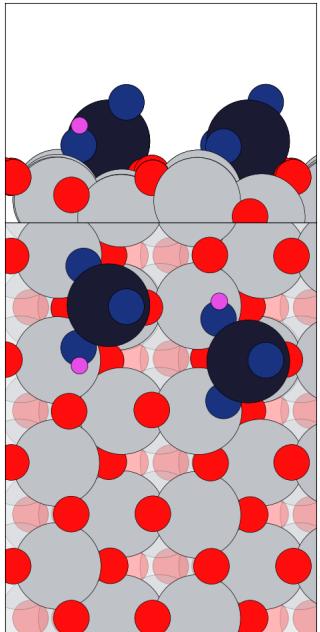


Method Vs Energy Order

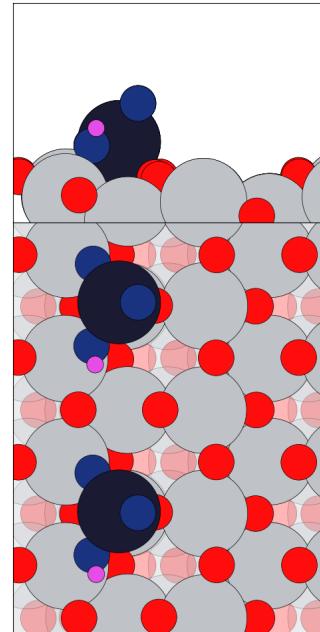
$M_2 = \text{GPAW (PW(500 eV),PBE,dzp,(2,2,1))}$ $M_3 = \text{GPAW (PW(500 eV),PBE,dzp,(2,2,1), U(4.0))}$



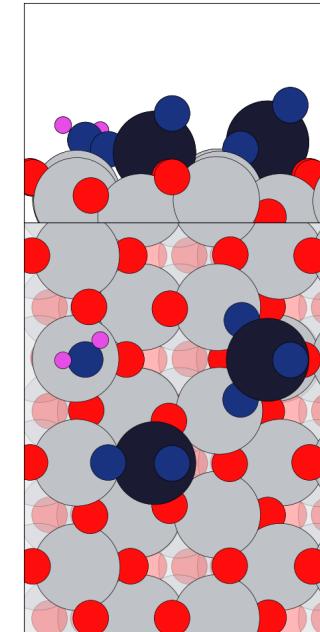
$M_2 : \Delta E = 0.050 \text{ eV}$



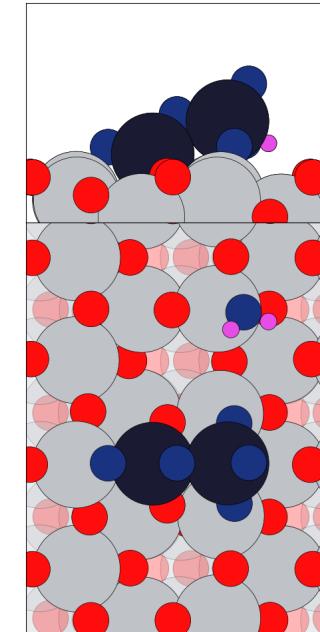
$M_2 : \Delta E = 0.000 \text{ eV}$



$M_2 : \Delta E = 0.082 \text{ eV}$



$M_2 : \Delta E = 0.394 \text{ eV}$



$M_2 : \Delta E = 0.293 \text{ eV}$

$M_3 : \Delta E = 0.000 \text{ eV}$

$M_3 : \Delta E = 0.002 \text{ eV}$

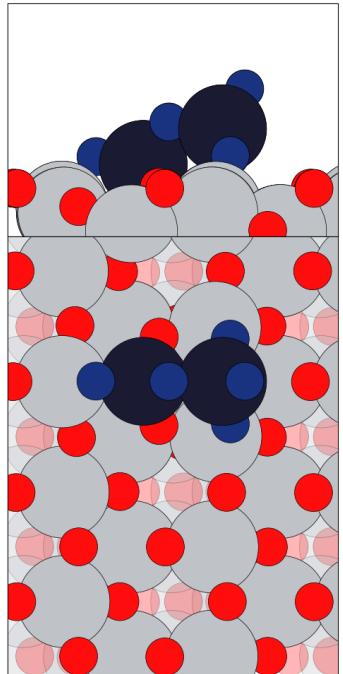
$M_3 : \Delta E = 0.006 \text{ eV}$

$M_3 : \Delta E = 0.068 \text{ eV}$

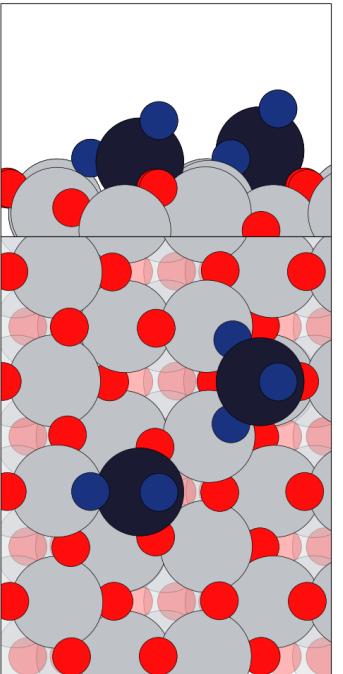
$M_3 : \Delta E = 0.078 \text{ eV}$

Method Vs Energy Order

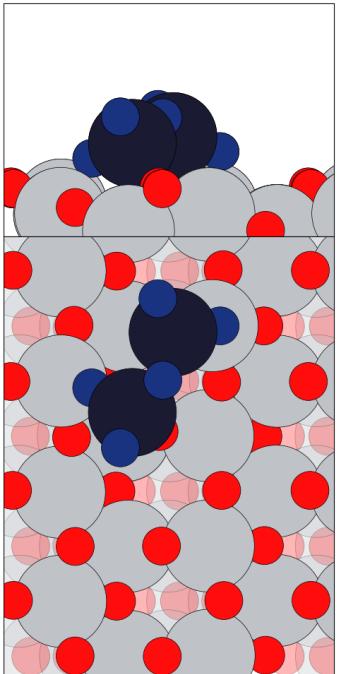
$M_2 = \text{GPAW (PW(500 eV),PBE,dzp,(2,2,1))}$ $M_3 = \text{GPAW (PW(500 eV),PBE,dzp,(2,2,1), U(4.0))}$



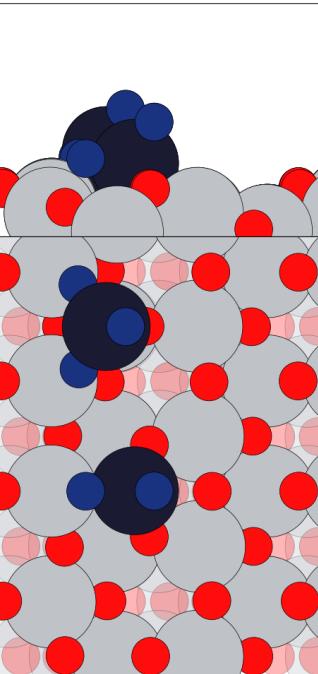
$M_2 : \Delta E = 0.000 \text{ eV}$



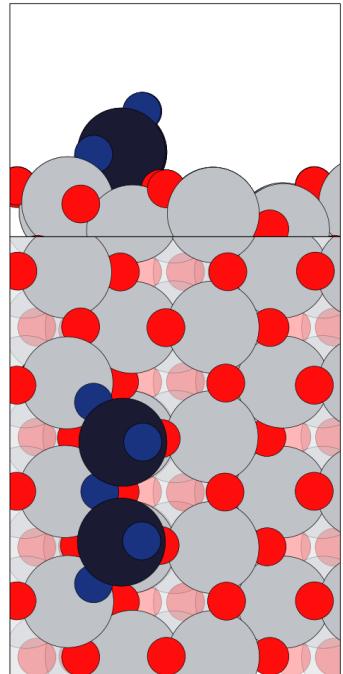
$M_2 : \Delta E = 0.249 \text{ eV}$



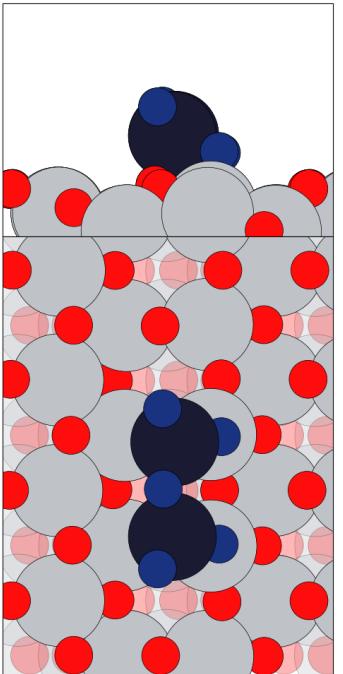
$M_2 : \Delta E = 0.669 \text{ eV}$



$M_2 : \Delta E = 0.776 \text{ eV}$



$M_2 : \Delta E = 0.865 \text{ eV}$



$M_2 : \Delta E = 0.107 \text{ eV}$

$M_3 : \Delta E = 0.000 \text{ eV}$

$M_3 : \Delta E = 0.131 \text{ eV}$

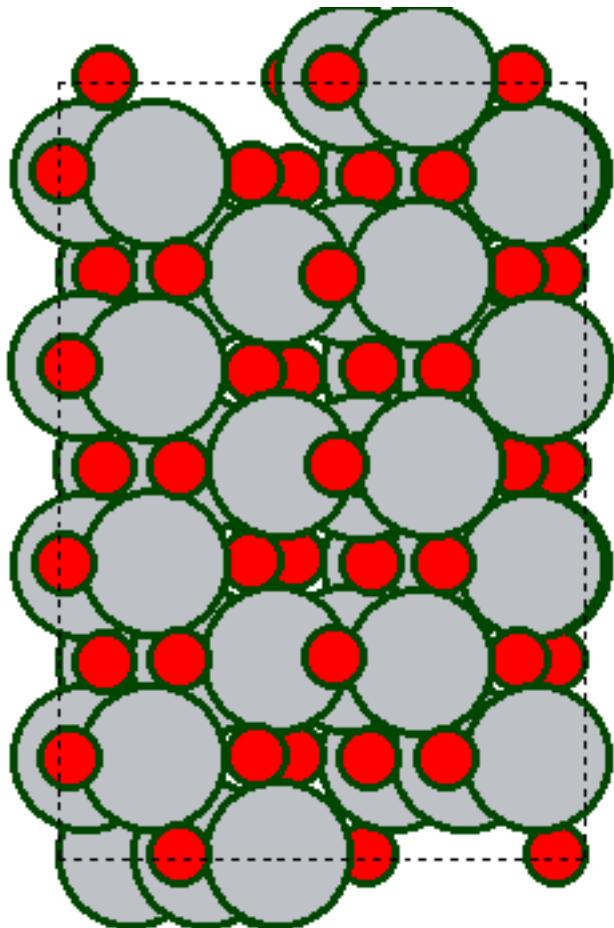
$M_3 : \Delta E = 0.257 \text{ eV}$

$M_3 : \Delta E = 0.127 \text{ eV}$

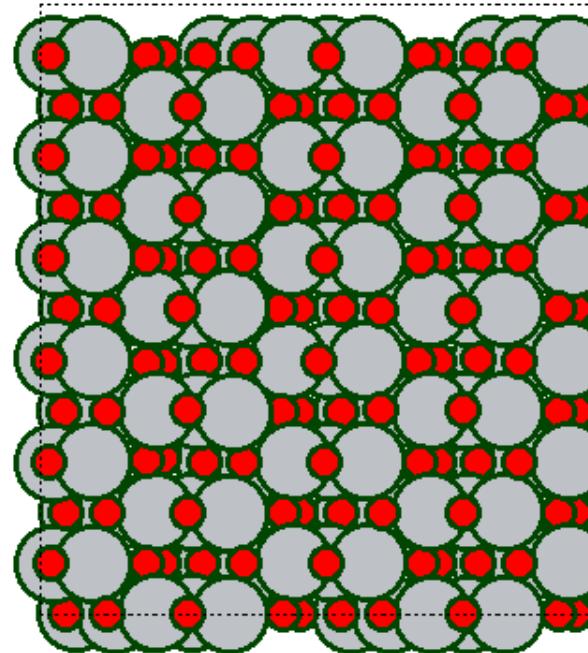
$M_3 : \Delta E = 0.326 \text{ eV}$

Super cells Used for Optimization

1×4 Super cell

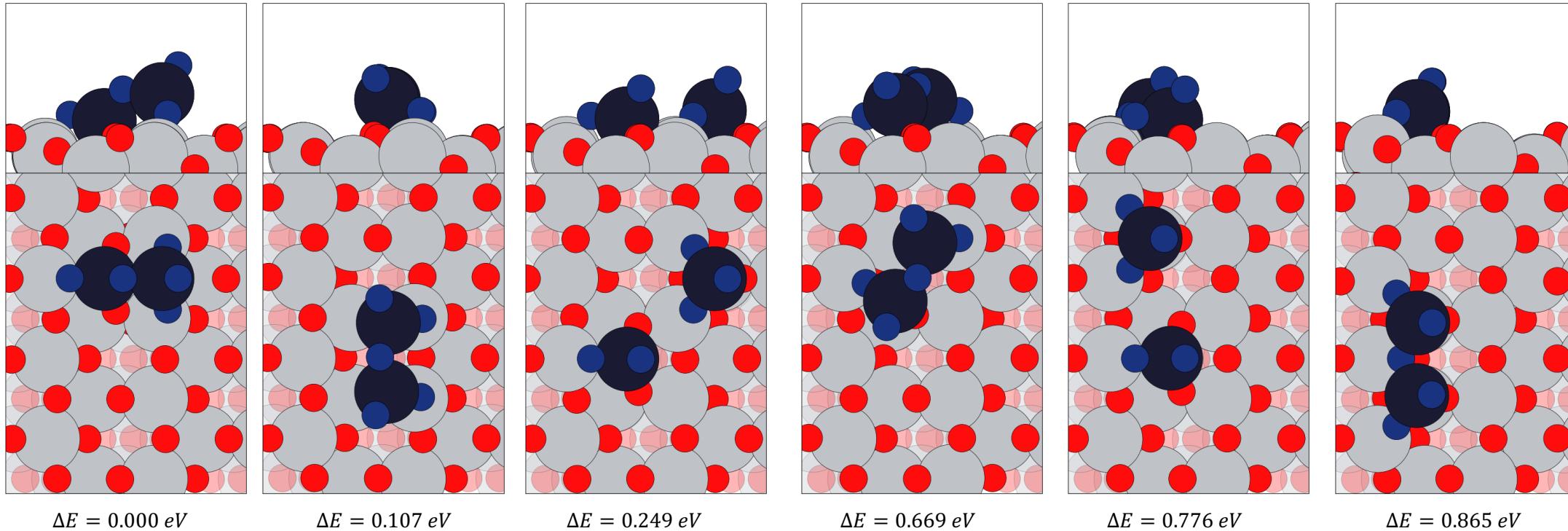


2×6 Super cell

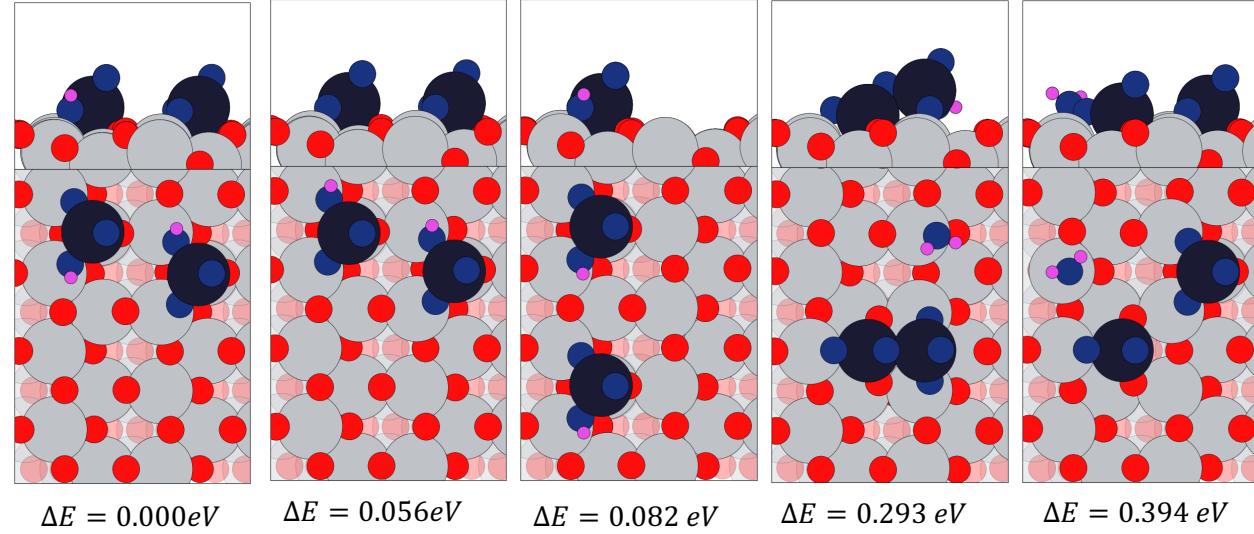


V_2O_5 O_v (1×4 Super cell)

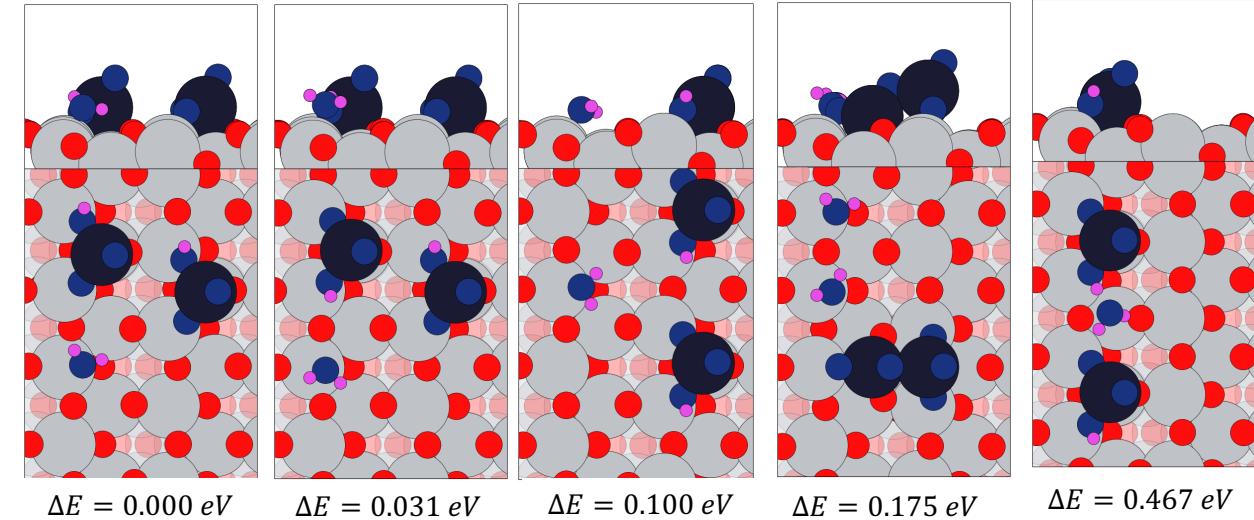
GPAW (PW(500 eV),PBE,dzp,(2,2,1))



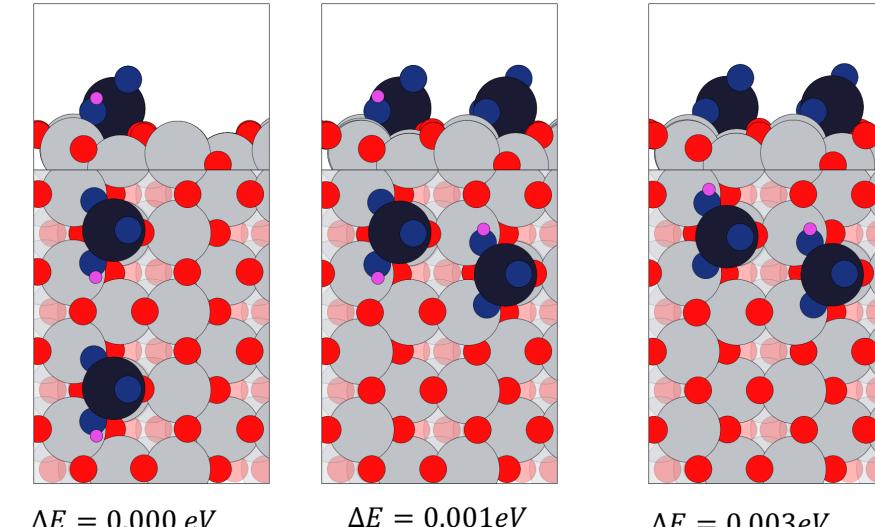
$\text{V}_2\text{O}_5 + \text{H}_2\text{O}$ with O_v (1×4 Super cell)



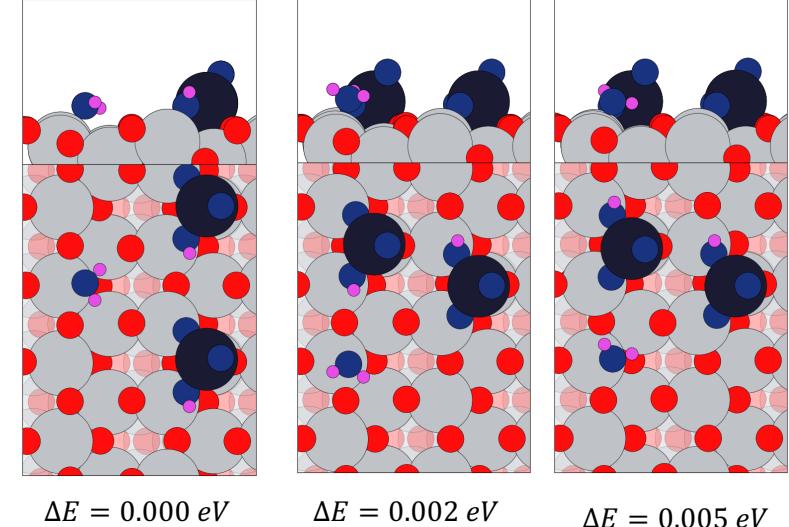
$\text{V}_2\text{O}_5 + 2 \text{ H}_2\text{O}$ with O_v (1×4 Super cell)



$\text{V}_2\text{O}_5 + \text{H}_2\text{O}$ with O_v (2×6 Super cell)

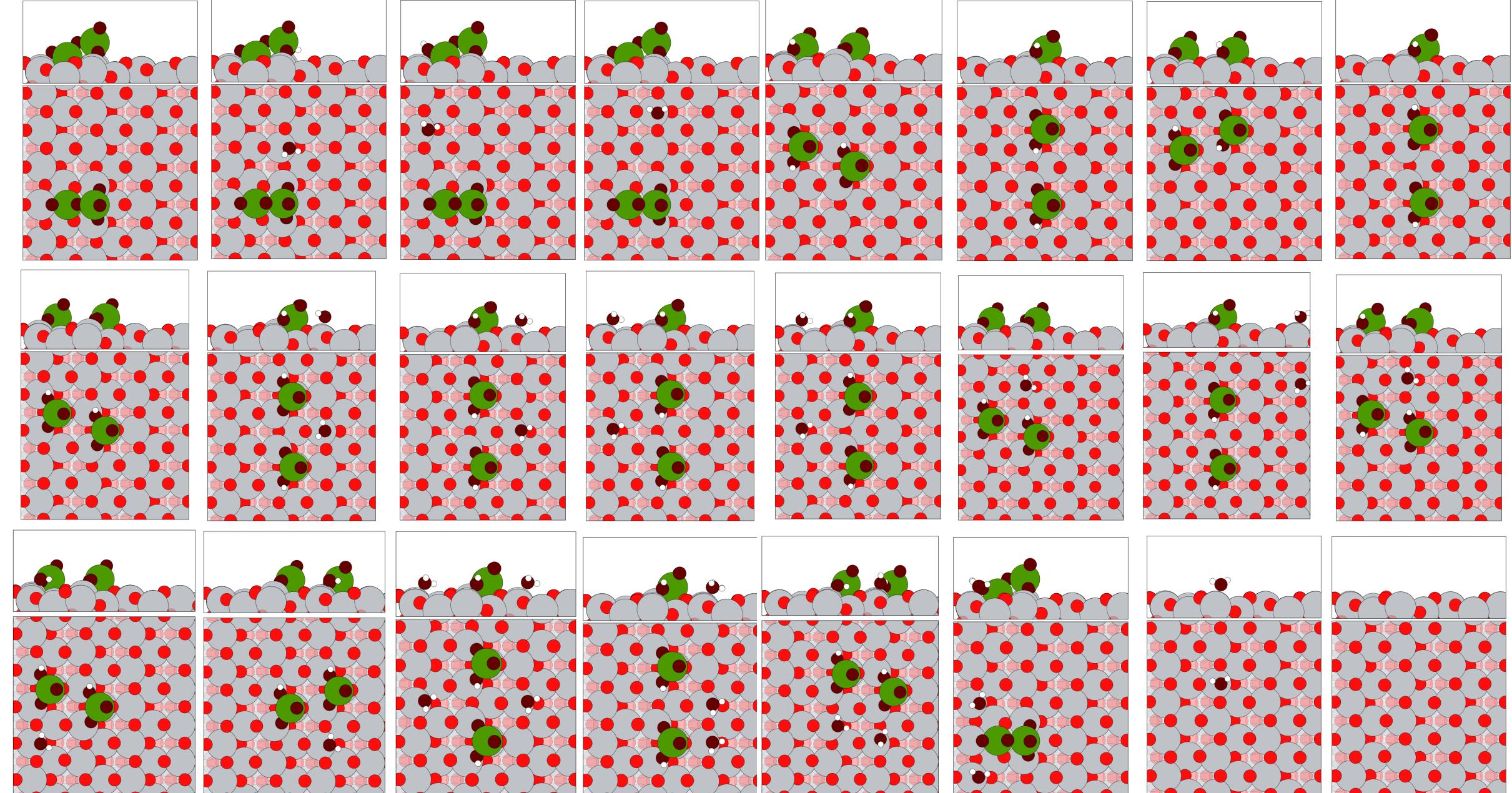


$\text{V}_2\text{O}_5 + 2 \text{ H}_2\text{O}$ with O_v (2×6 Super cell)

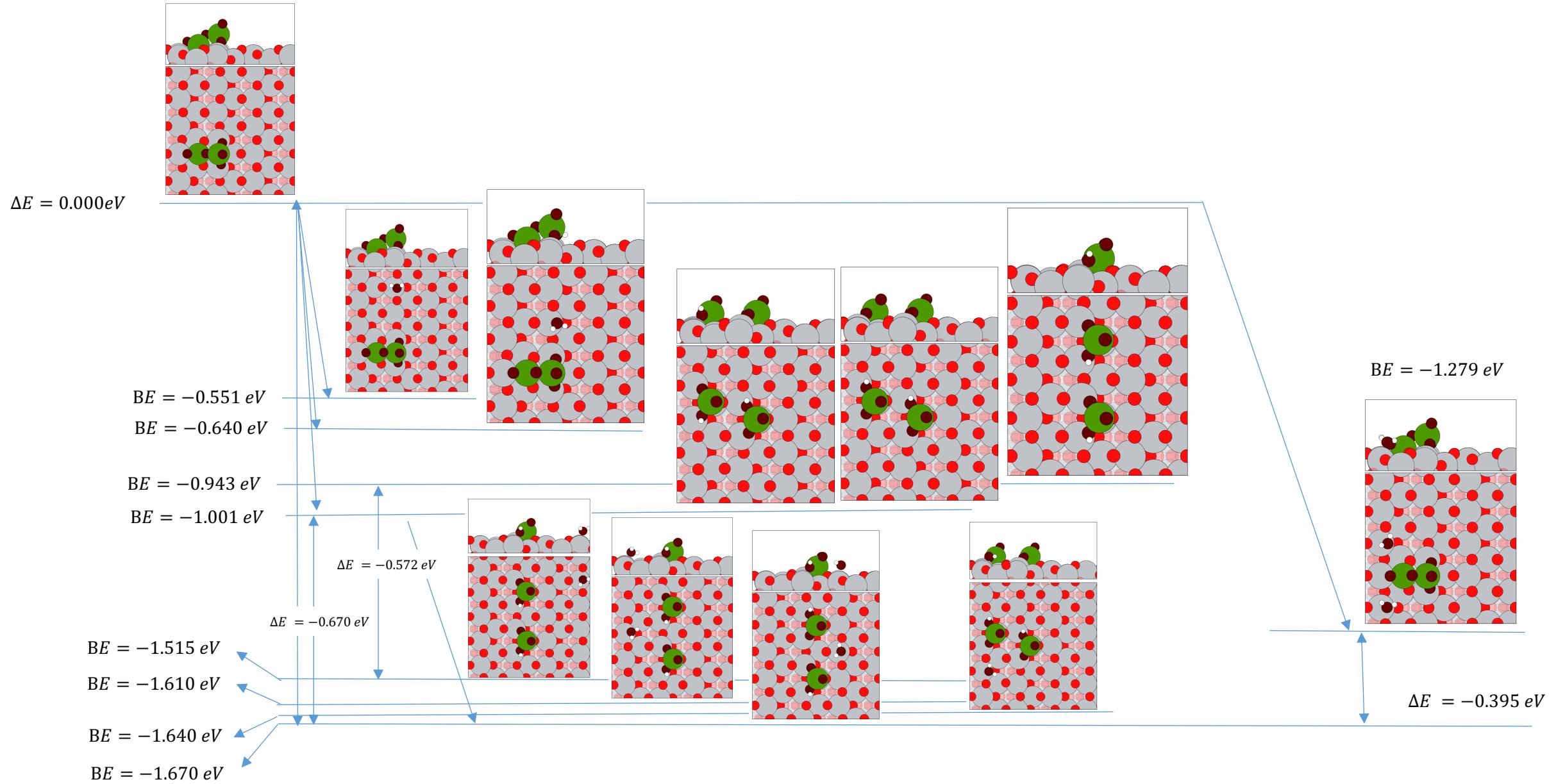


For 2×6 Super cell
force converged up to
0.055 eV/Ang during
optimization

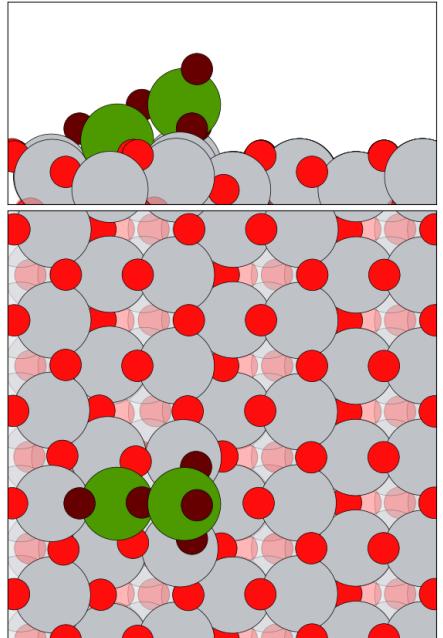
Binding Energy of H₂O on V₂O₅/TiO₂ (2×6 super cell)



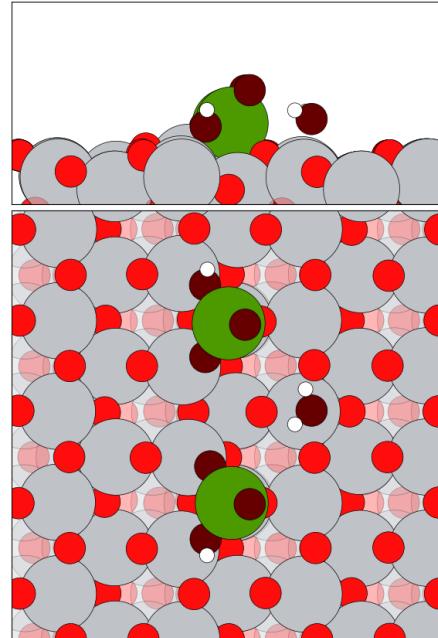
Binding Energy of H₂O on V₂O₅/TiO₂ (6×2 super cell)



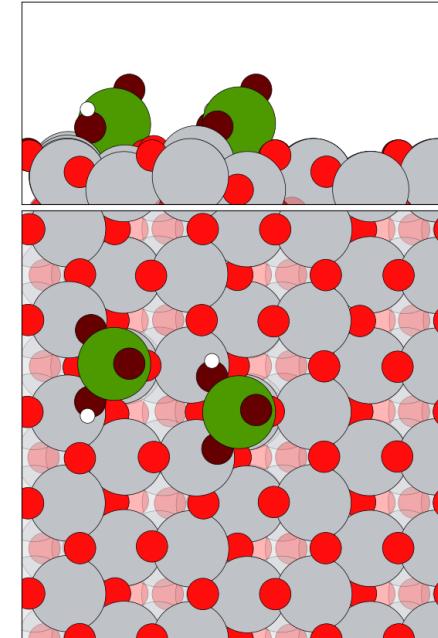
Before



During



After



GPAW and CP2K

GPAW

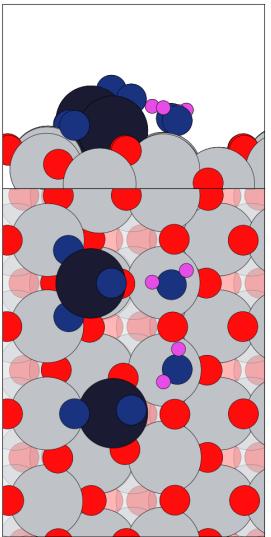
Mode = PW

E_cut = 500 eV for plane wave

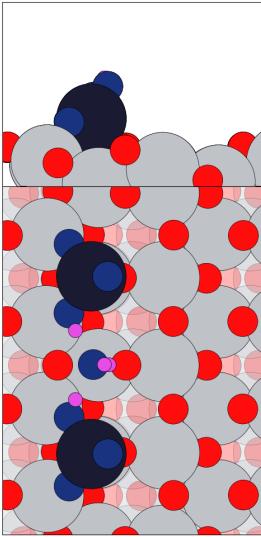
XC = PBE

U_corr (Hubbard term) = 4.0 eV

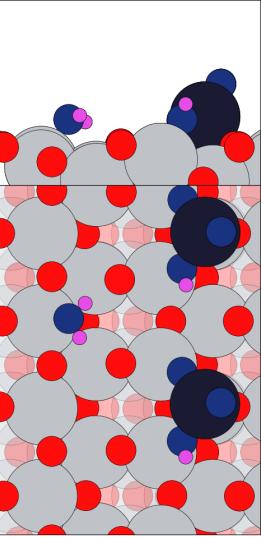
F_cut = 0.025 eV/Ang



I1: $\Delta E = 0.00 \text{ eV}$



I2: $\Delta E = 0.12 \text{ eV}$



I3: $\Delta E = 0.130 \text{ eV}$

CP2K

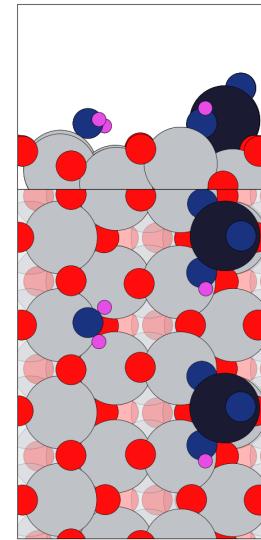
Mode = GPW (gaussian and plane wave method)

E_cut = 400 Ry for plane wave

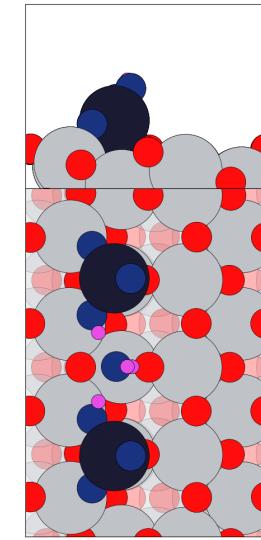
XC = PBE

Dispersion correction = DFTD3 (PBE functional)

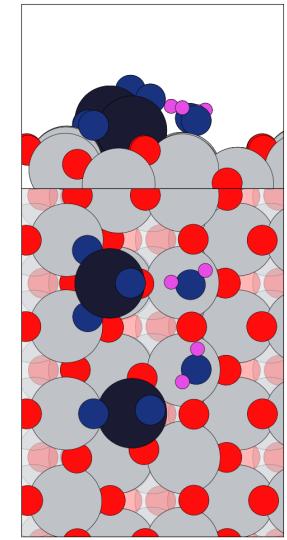
F_cut = 0.023 eV/Ang



I1: $\Delta E = 0.00 \text{ eV}$

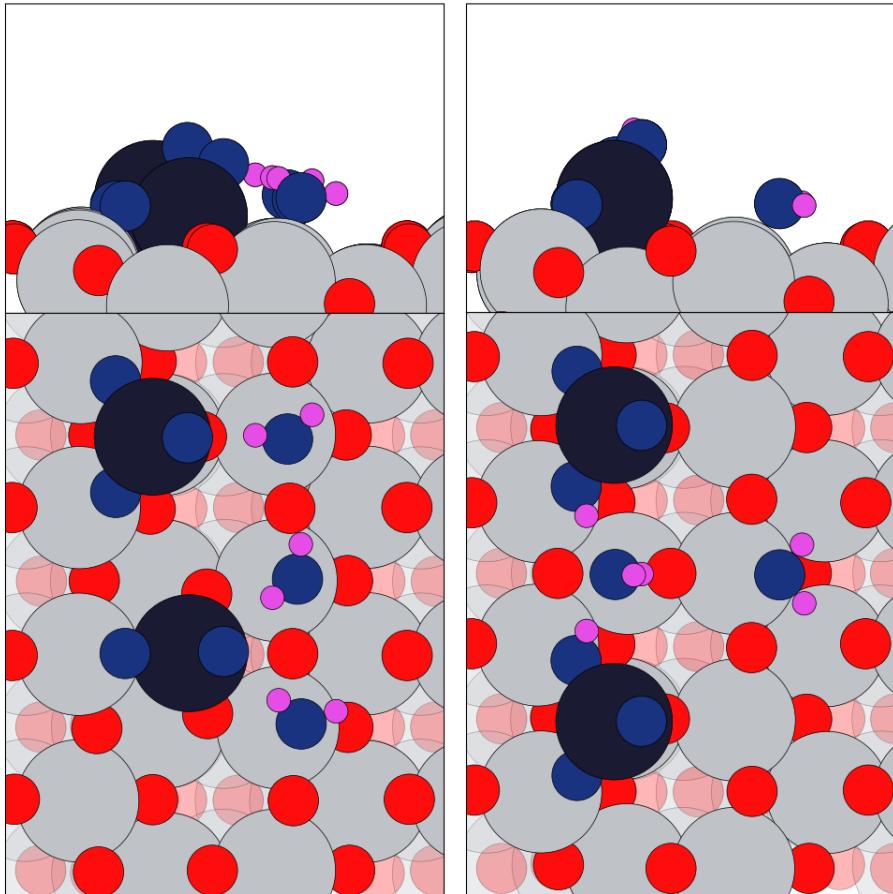
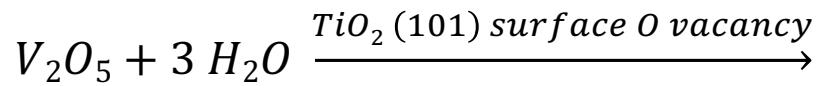


I2: $\Delta E = 0.13 \text{ eV}$



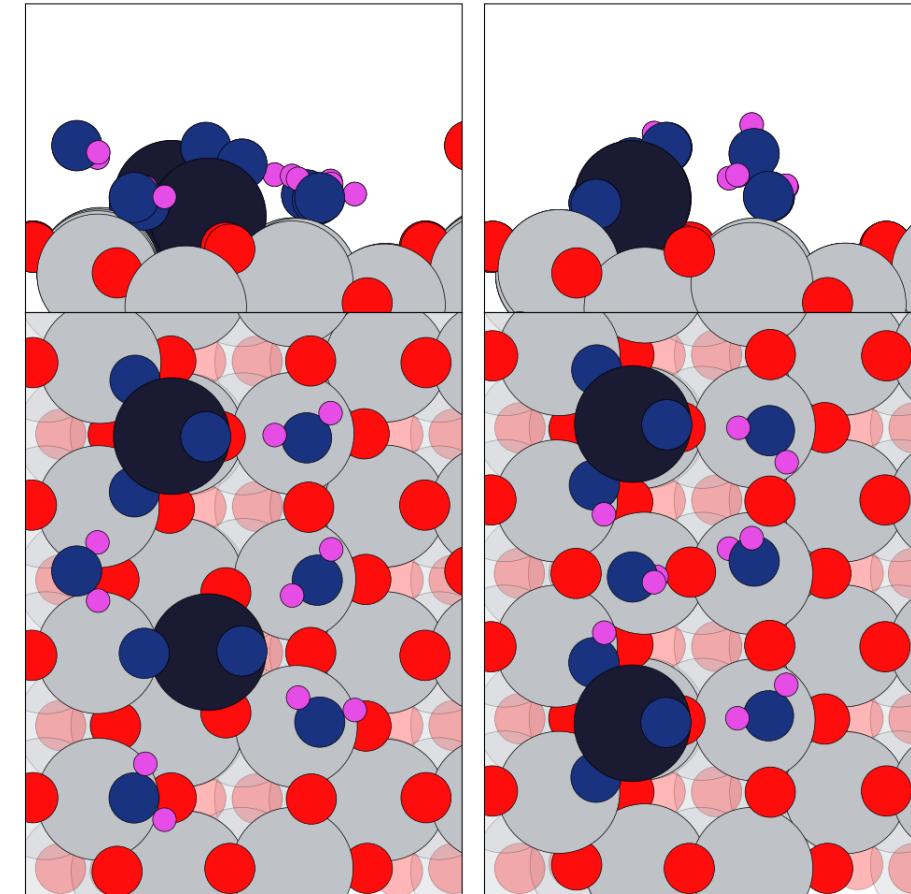
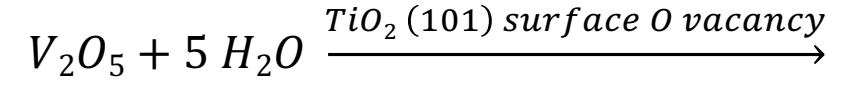
I3: $\Delta E = 0.71 \text{ eV}$

V_2O_5 Clusters with O_v (1by4 Super cell)



|1: $\Delta E = 0.000 \text{ eV}$

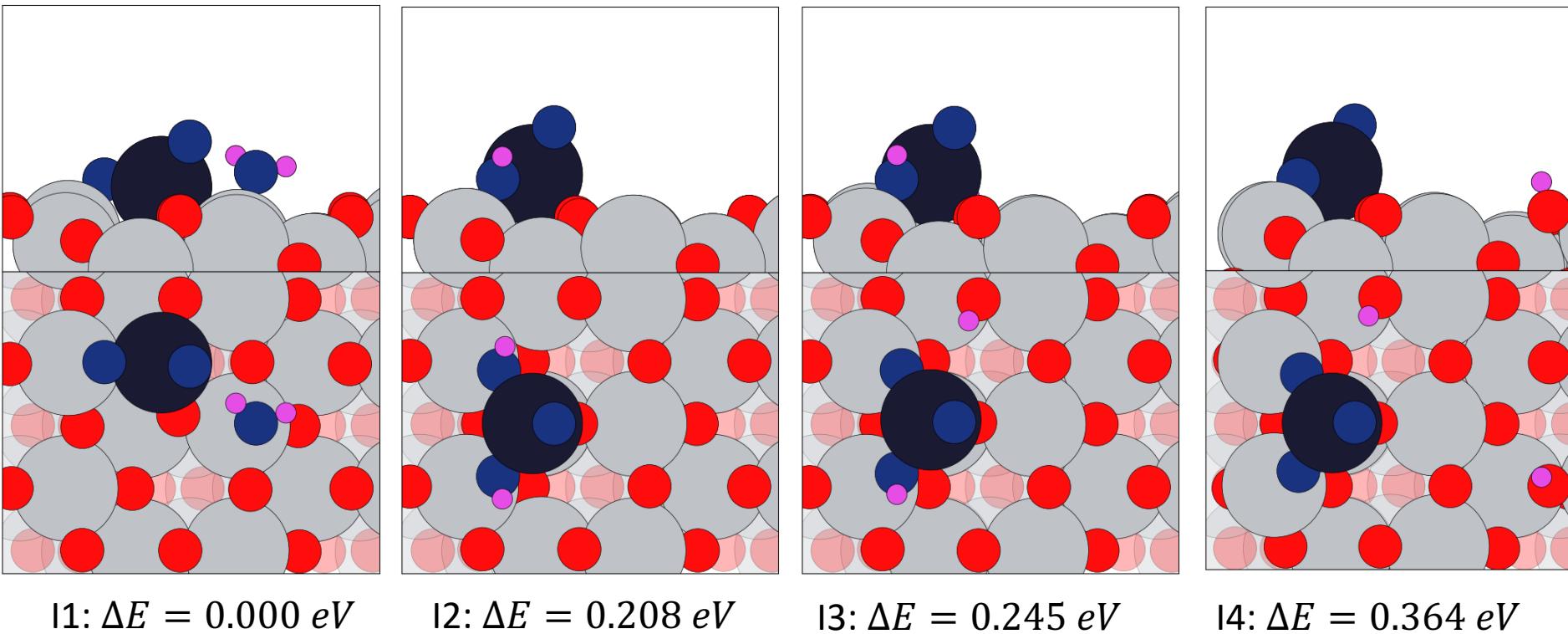
|2: $\Delta E = 0.272 \text{ eV}$



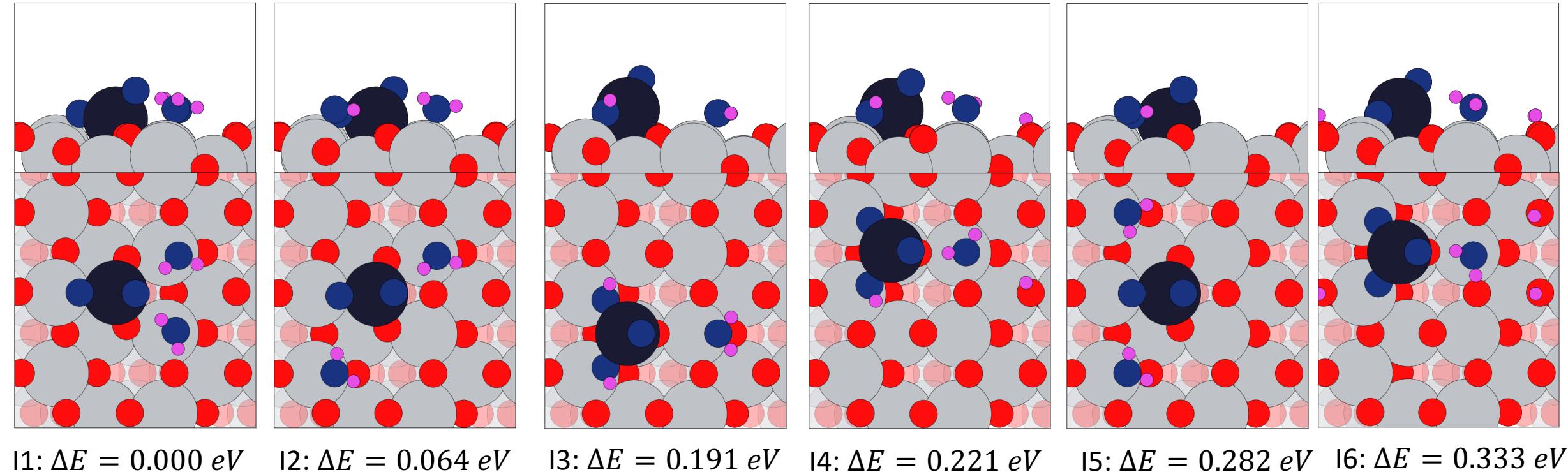
|1: $\Delta E = 0.000 \text{ eV}$

|2: $\Delta E = 0.141 \text{ eV}$

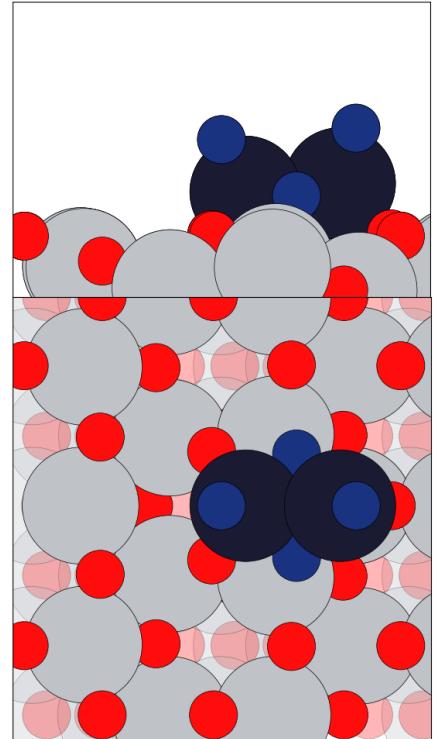
$\text{VO}_2 + \text{H}_2\text{O}$ Clusters (1by2 Super cell)



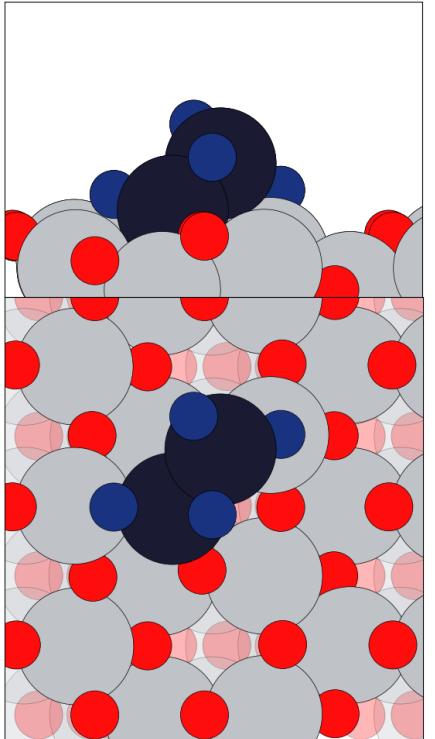
$\text{VO}_2 + 2\text{H}_2\text{O}$ Clusters (1by3 Super cell)



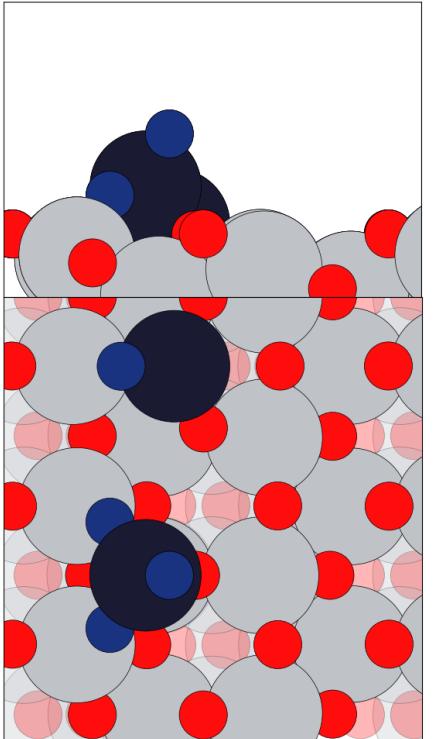
V_2O_4 Clusters (1by3 Super cell)



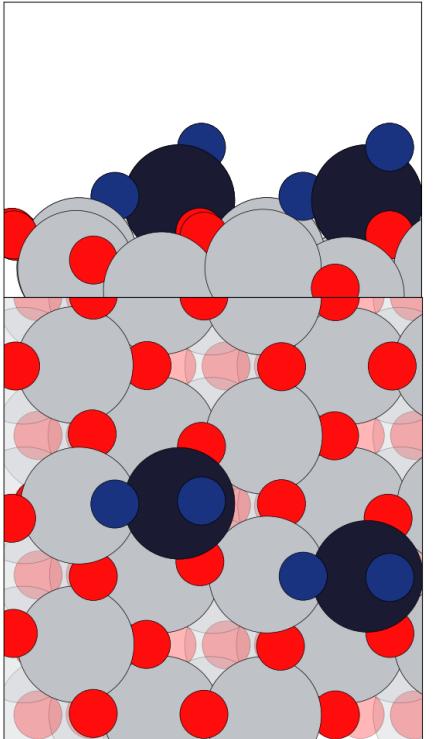
I1: $\Delta E = 0.000 \text{ eV}$



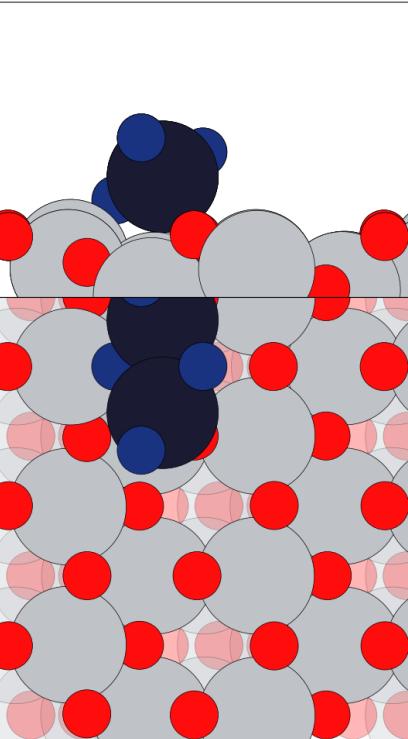
I2: $\Delta E = 0.207 \text{ eV}$



I3: $\Delta E = 0.290 \text{ eV}$

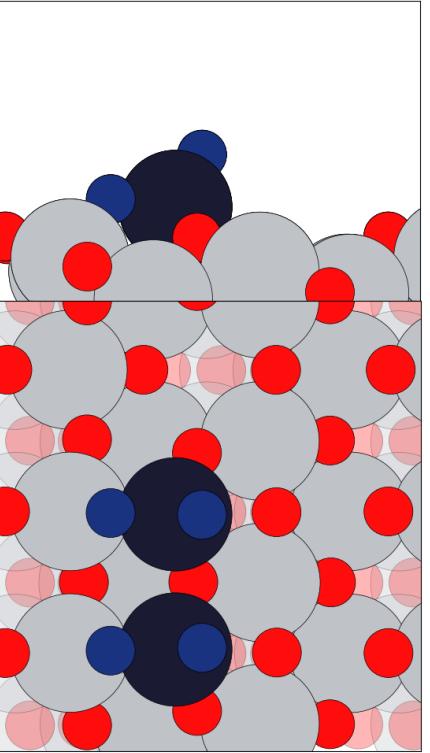
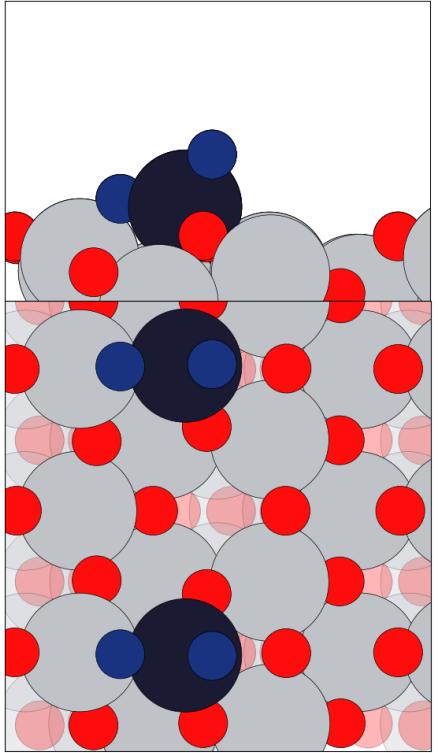


I4: $\Delta E = 0.466 \text{ eV}$



I5: $\Delta E = 0.814 \text{ eV}$

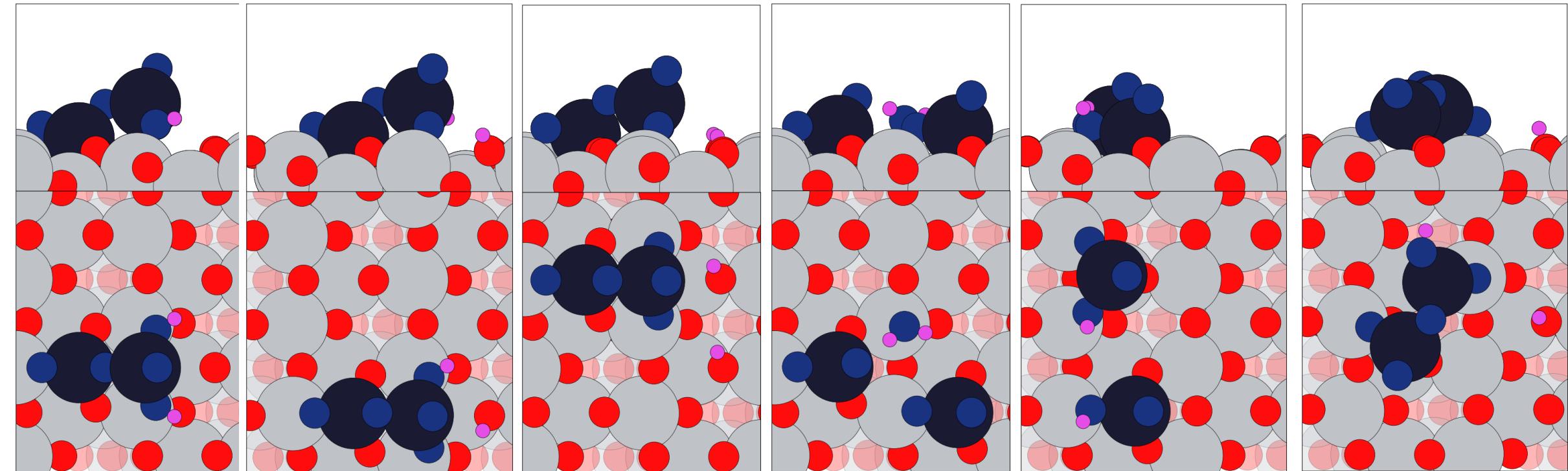
V_2O_4 Clusters (1by3 Super cell)



I6: $\Delta E = 1.087 \text{ eV}$

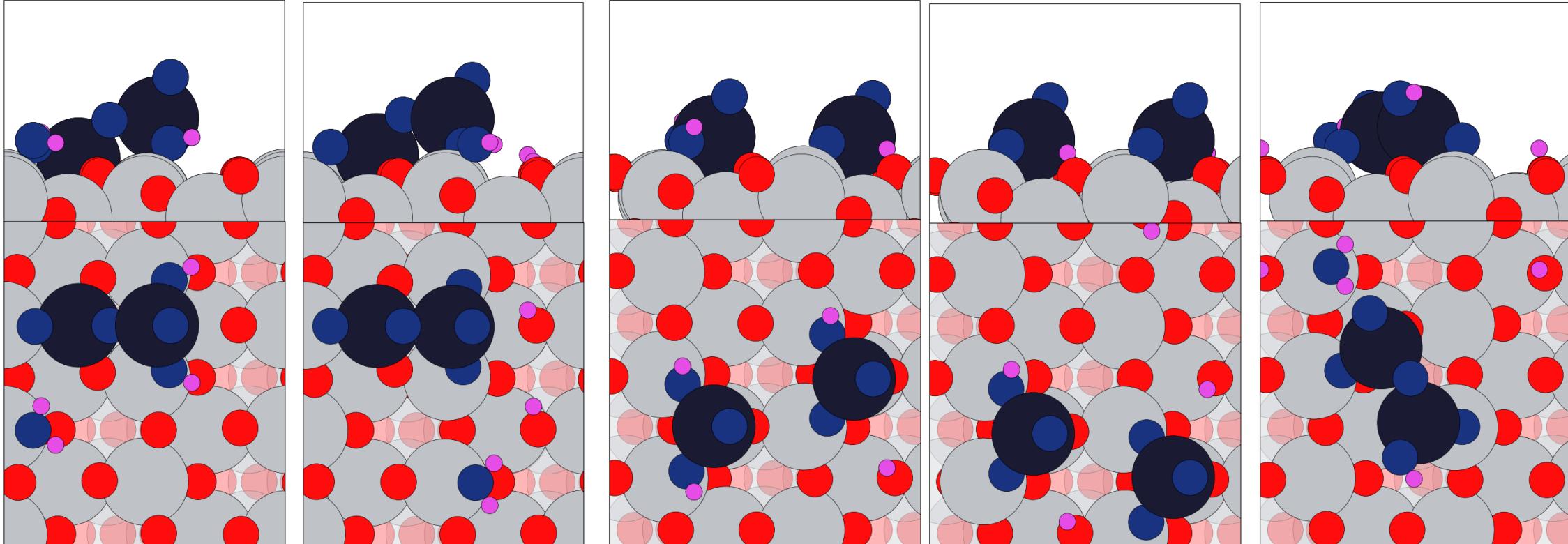
I7: $\Delta E = 1.101 \text{ eV}$

$\text{V}_2\text{O}_4 + \text{H}_2\text{O}$ Clusters (1by3 Super cell)



I1: $\Delta E = 0.000 \text{ eV}$ I2: $\Delta E = 0.221 \text{ eV}$ I3: $\Delta E = 0.415 \text{ eV}$ I4: $\Delta E = 0.568 \text{ eV}$ I5: $\Delta E = 0.615 \text{ eV}$ I6: $\Delta E = 0.760 \text{ eV}$

$\text{V}_2\text{O}_4 + 2\text{H}_2\text{O}$ Clusters (1by3 Super cell)



I1: $\Delta E = 0.000 \text{ eV}$

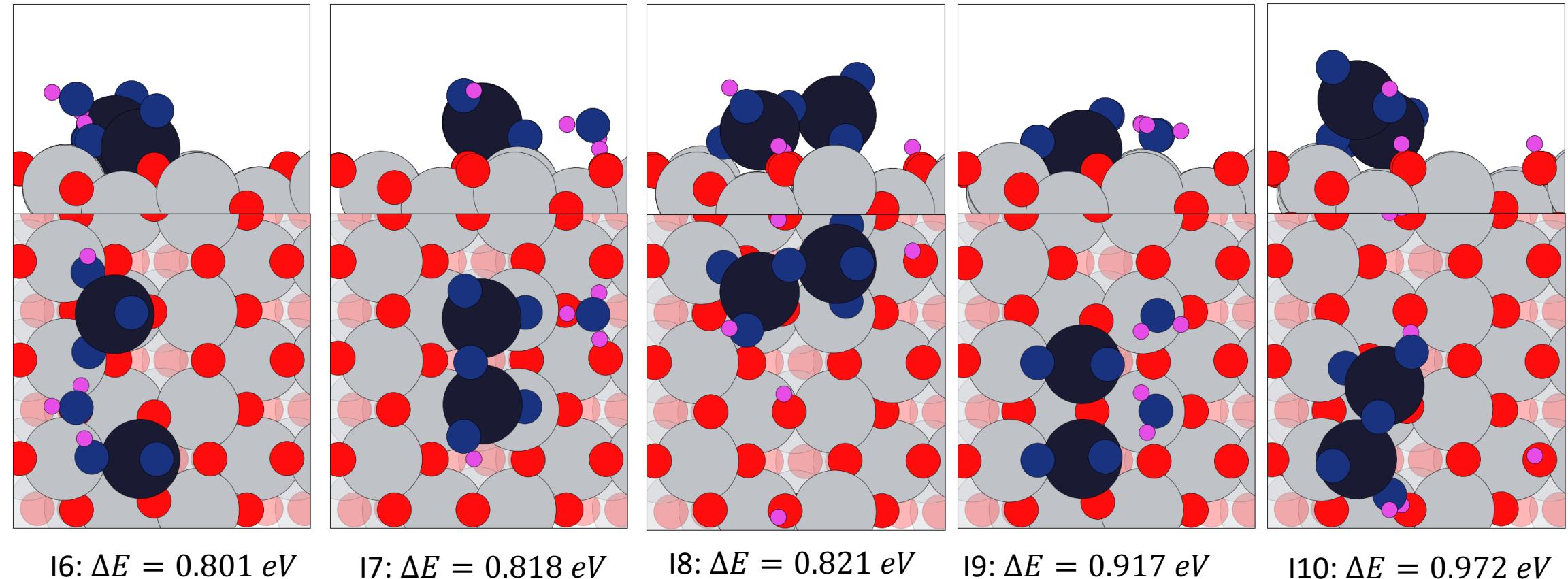
I2: $\Delta E = 0.436 \text{ eV}$

I3: $\Delta E = 0.597 \text{ eV}$

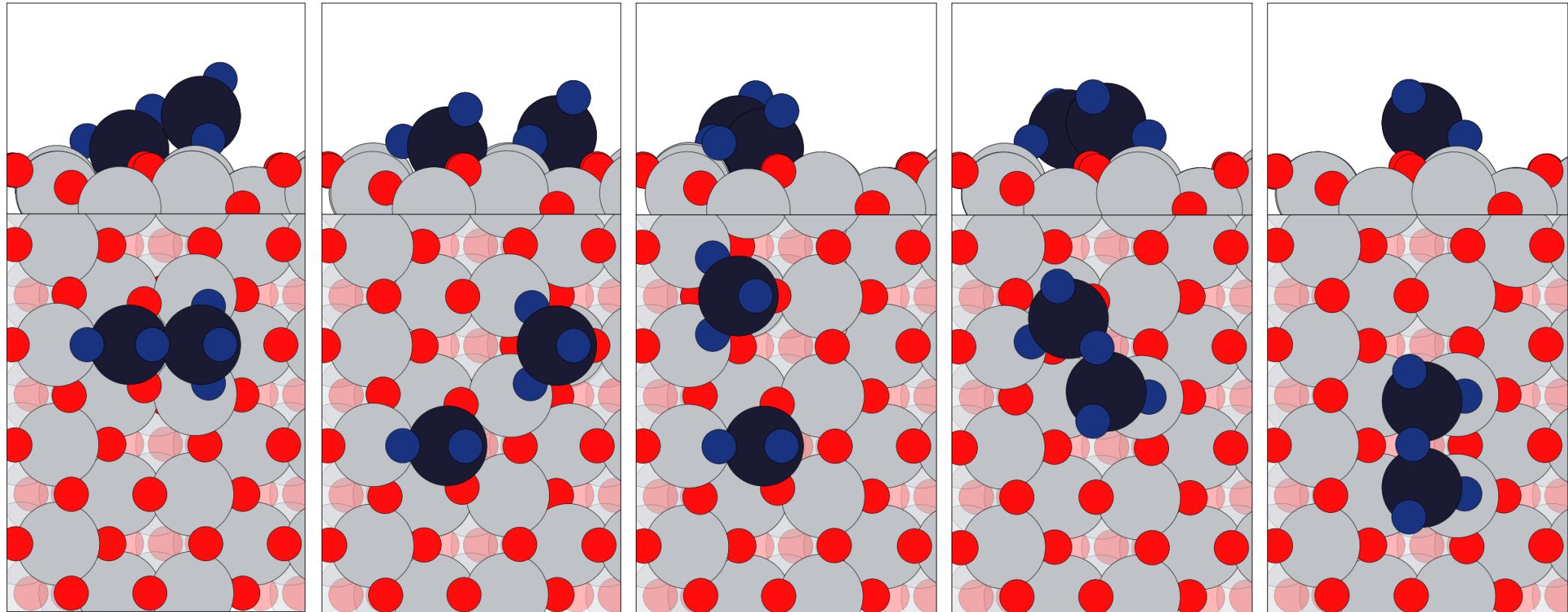
I4: $\Delta E = 0.642 \text{ eV}$

I5: $\Delta E = 0.736 \text{ eV}$

$\text{V}_2\text{O}_4 + 2\text{H}_2\text{O}$ Clusters (1by3 Super cell)



V_2O_5 Clusters (1by4 Super cell)



I1: $\Delta E = 0.000 \text{ eV}$

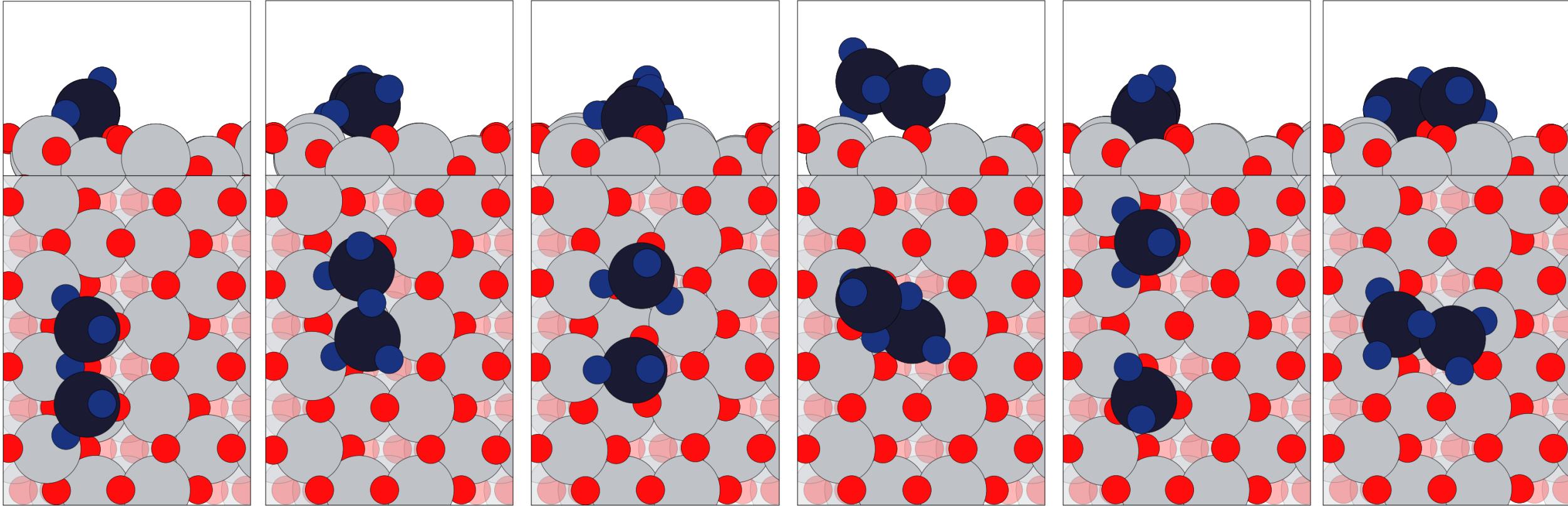
I2: $\Delta E = 0.226 \text{ eV}$

I3: $\Delta E = 0.290 \text{ eV}$

I4: $\Delta E = 0.409 \text{ eV}$

I5: $\Delta E = 0.414 \text{ eV}$

V_2O_5 Clusters (1by4 Super cell)



I6: $\Delta E = 0.600 \text{ eV}$

I7: $\Delta E = 1.016 \text{ eV}$

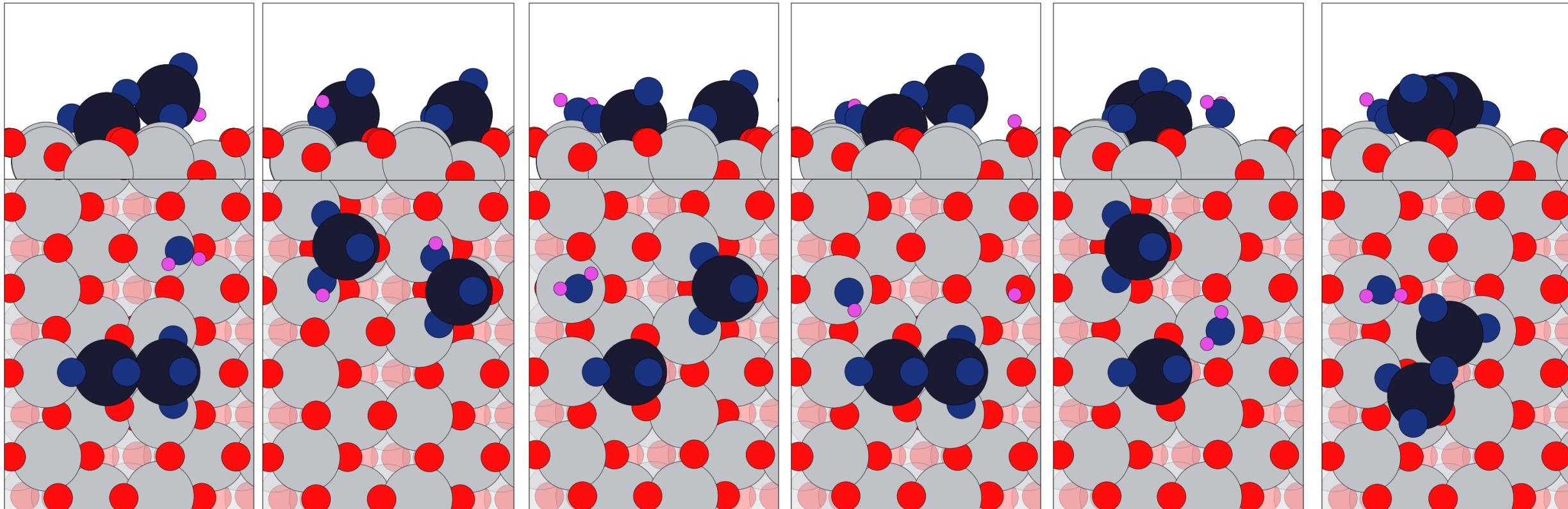
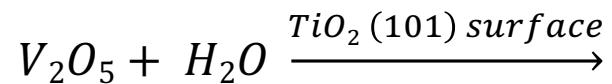
I8: $\Delta E = 1.231 \text{ eV}$

I9: $\Delta E = 1.350 \text{ eV}$

I10: $\Delta E = 1.430 \text{ eV}$

I11: $\Delta E = 1.481 \text{ eV}$

V_2O_5 Clusters (1by4 Super cell)



I1: $\Delta E = 0.000 \text{ eV}$

I2: $\Delta E = 0.044 \text{ eV}$

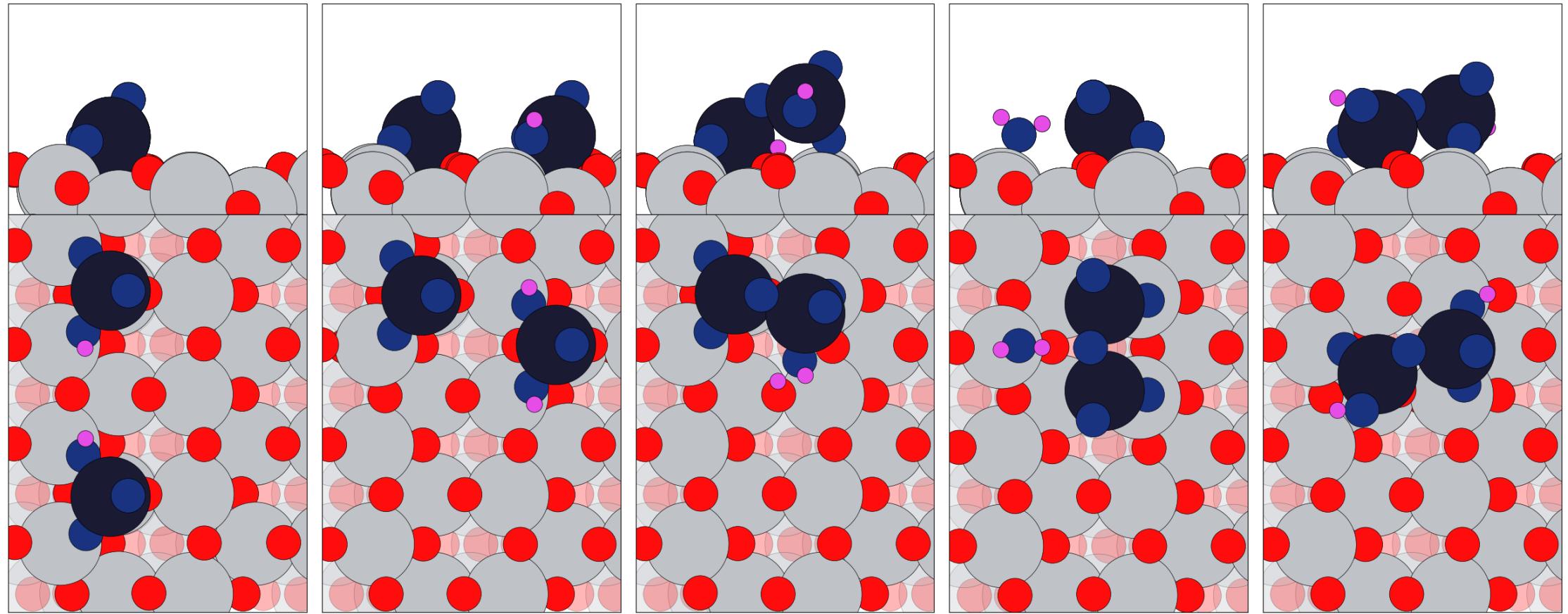
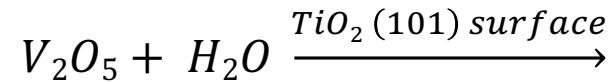
I3: $\Delta E = 0.072 \text{ eV}$

I4: $\Delta E = 0.132 \text{ eV}$

I5: $\Delta E = 0.155 \text{ eV}$

I6: $\Delta E = 0.221 \text{ eV}$

V_2O_5 Clusters (1by4 Super cell)



I7: $\Delta E = 0.260 \text{ eV}$

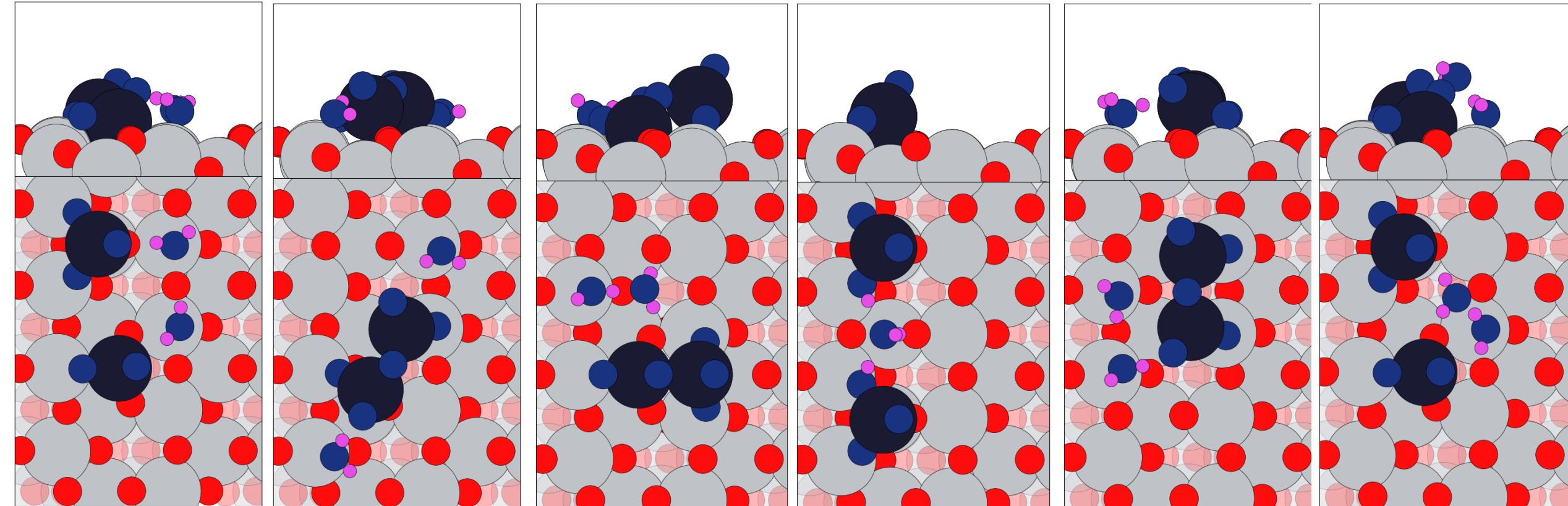
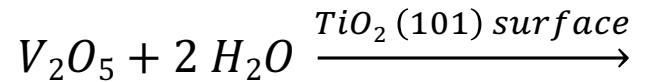
I8: $\Delta E = 0.287 \text{ eV}$

I9: $\Delta E = 0.335 \text{ eV}$

I10: $\Delta E = 0.371 \text{ eV}$

I11: $\Delta E = 0.452 \text{ eV}$

V_2O_5 Clusters (1by4 Super cell)



I1: $\Delta E = 0.000 \text{ eV}$

I2: $\Delta E = 0.145 \text{ eV}$

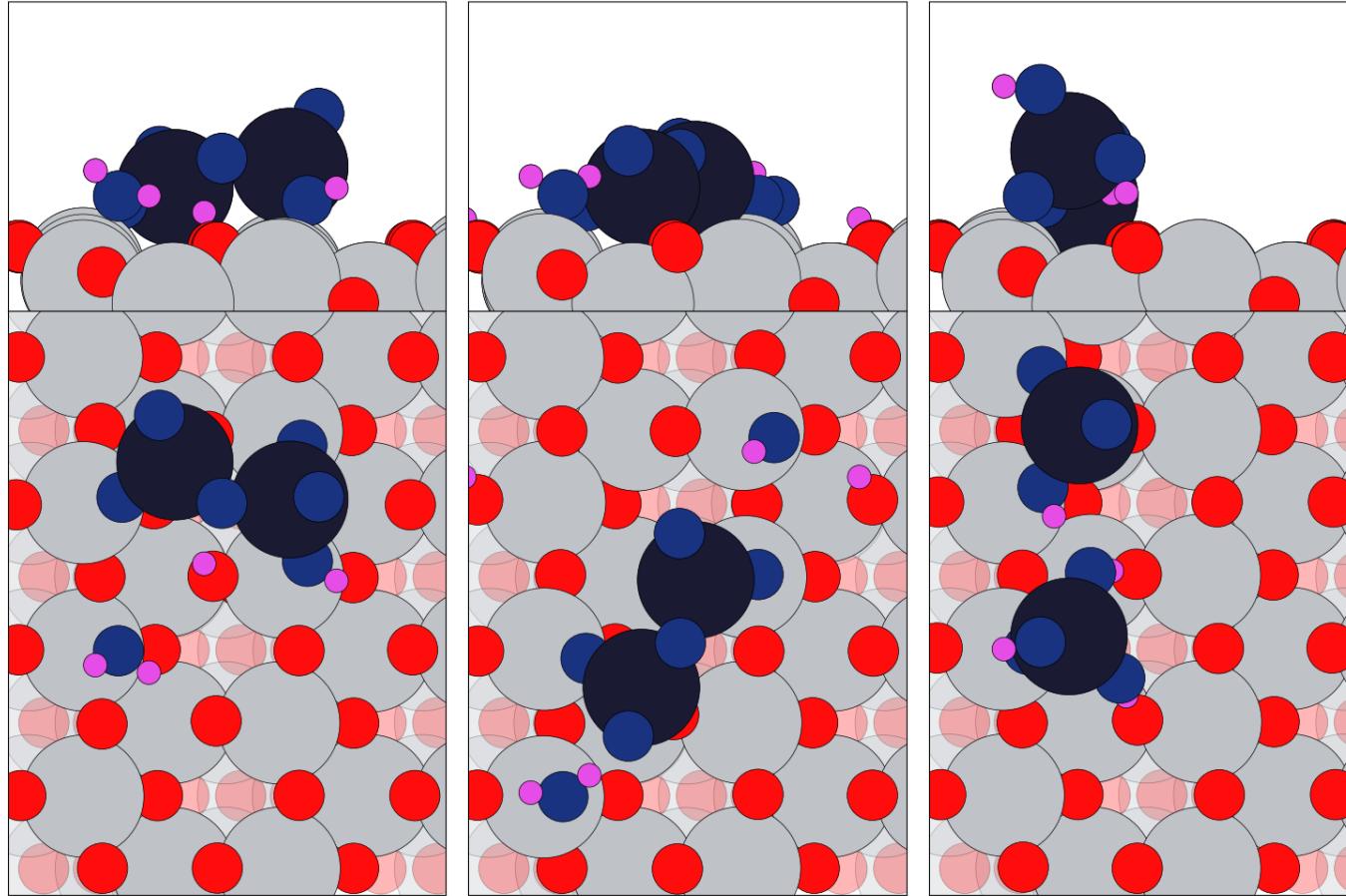
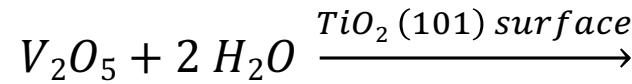
I3: $\Delta E = 0.196 \text{ eV}$

I4: $\Delta E = 0.254 \text{ eV}$

I5: $\Delta E = 0.341 \text{ eV}$

I6: $\Delta E = 0.352 \text{ eV}$

V_2O_5 Clusters (1by4 Super cell)

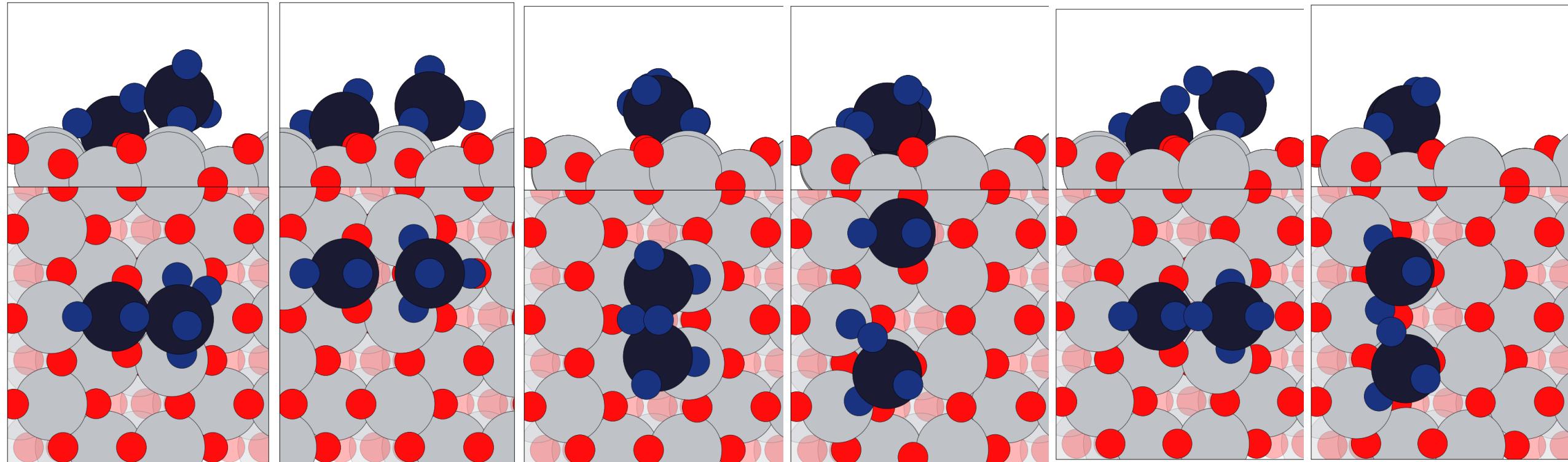


I7: $\Delta E = 0.399 \text{ eV}$

I8: $\Delta E = 0.462 \text{ eV}$

I9: $\Delta E = 0.684 \text{ eV}$

V_2O_6 Clusters (1by3 Super cell)



I1: $\Delta E = 0.00 \text{ eV}$

I2: $\Delta E = 0.204 \text{ eV}$

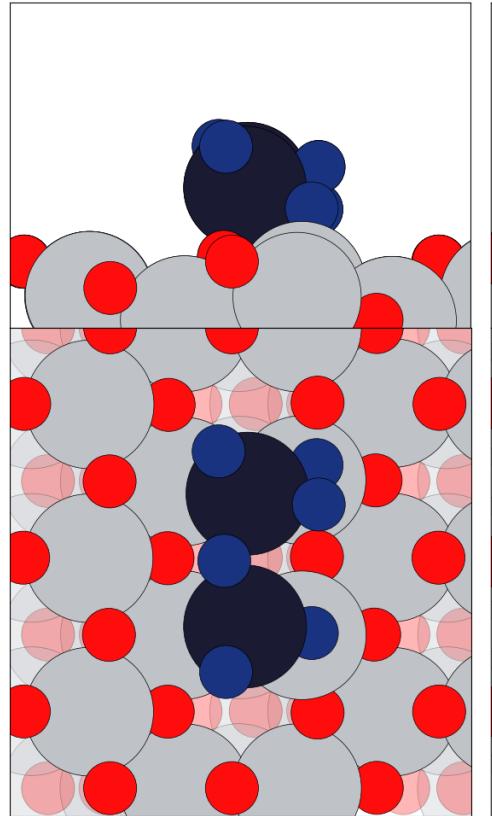
I3: $\Delta E = 0.254 \text{ eV}$

I4: $\Delta E = 0.386 \text{ eV}$

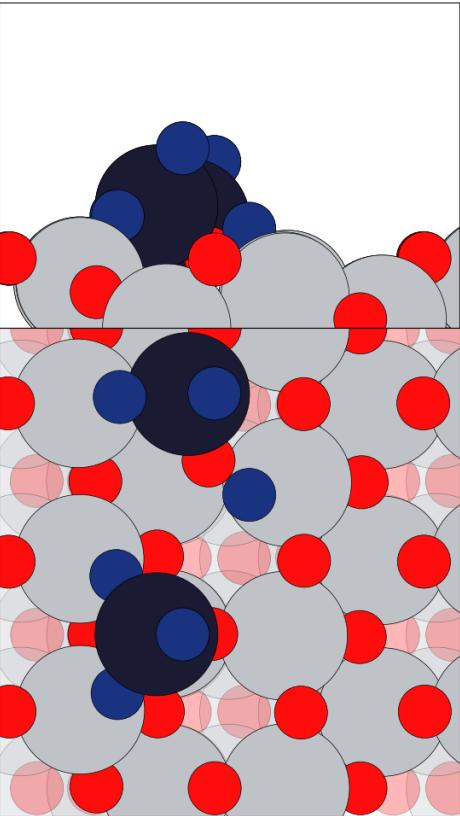
I5: $\Delta E = 0.388 \text{ eV}$

I6: $\Delta E = 0.398 \text{ eV}$

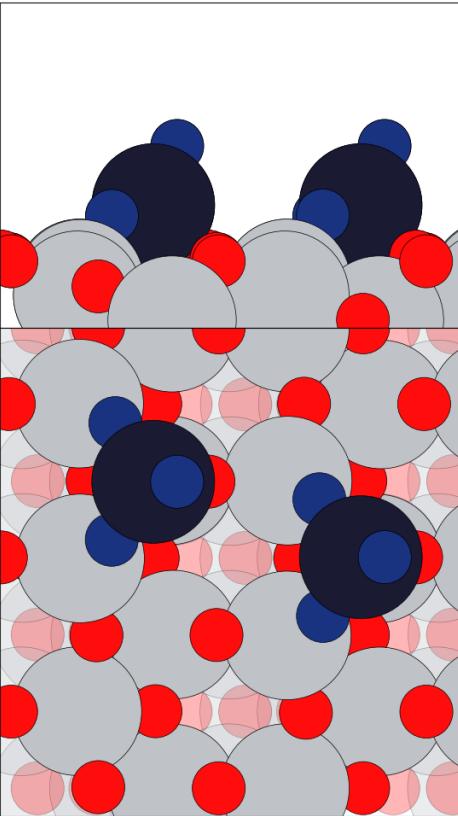
V_2O_6 Clusters (1by3 Super cell)



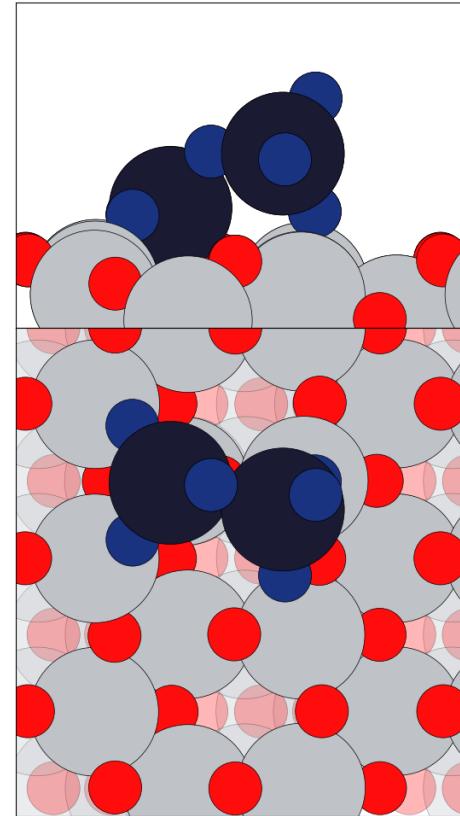
I7: $\Delta E = 0.479 \text{ eV}$



I8: $\Delta E = 0.496 \text{ eV}$

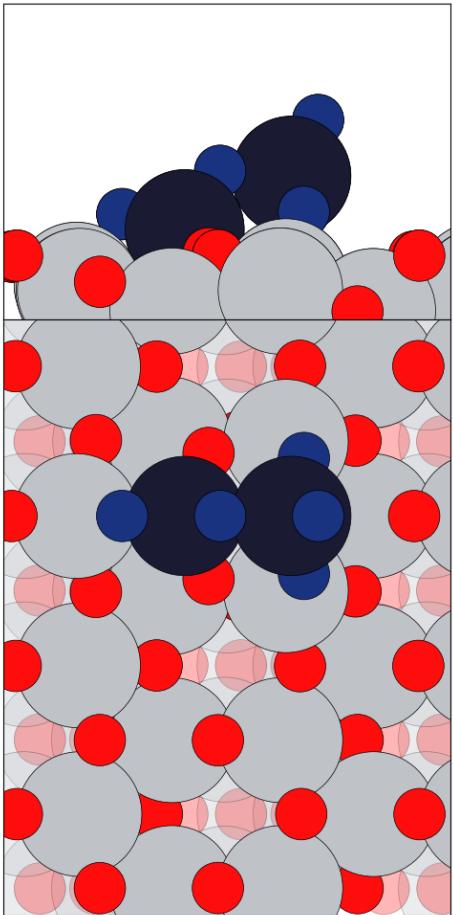


I9: $\Delta E = 1.373 \text{ eV}$



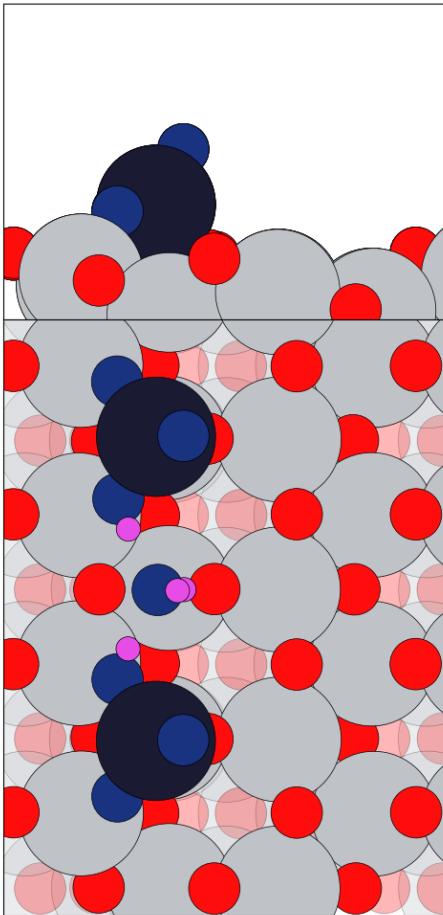
I10: $\Delta E = 1.912 \text{ eV}$

Before H₂O exposer



Global minimum

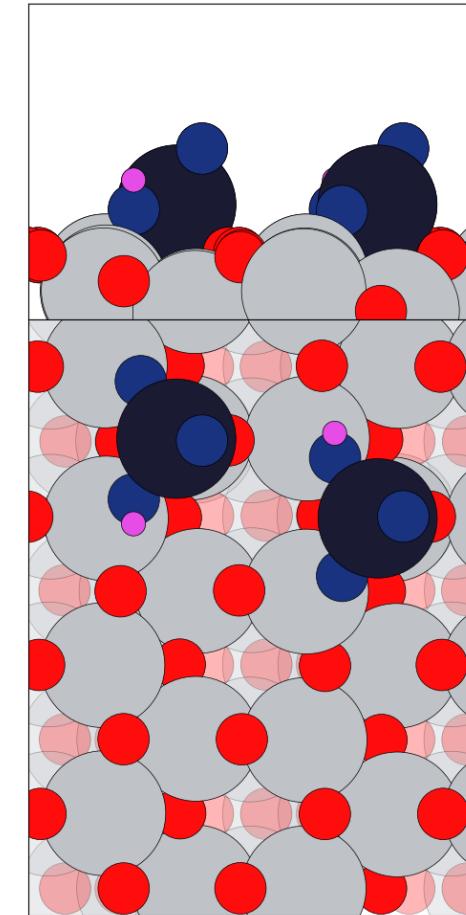
During H₂O exposer



I2: $\Delta E = 0.100 \text{ eV}$

This becomes GM if we have
more than 2 H₂O

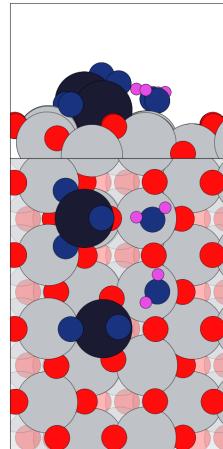
After H₂O exposer



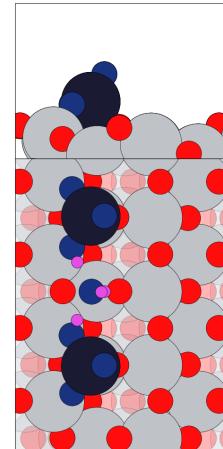
Global minimum

U_{eff} (eV)	Stoichiometric surface ΔE (eV) U_{eff} for only V	Reduced surface ΔE (eV) U_{eff} for both V & Ti	Reduced surface ΔE (eV) U_{eff} for only Ti	Stoichiometric surface ΔE (eV) U_{eff} for only Ti
4.0	0.128	0.078	0.103	0.254
3.0	0.136	0.075		
2.0	0.142	0.075		

I1



I2

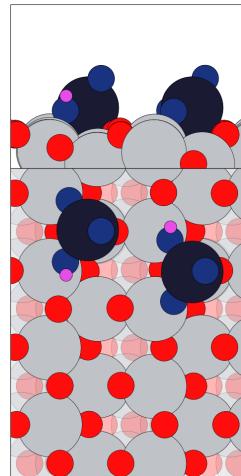


$$\Delta E = EI_2 - EI_1$$

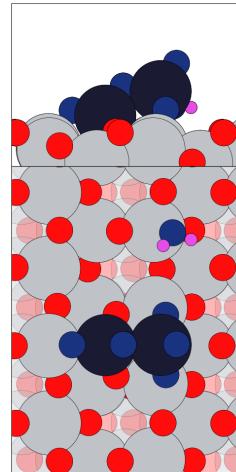
$$\Delta E = EI_2 - EI_1$$

U_{eff} (eV)	Stoichiometric surface ΔE (eV) U_{eff} for only V	Reduced surface ΔE (eV) U_{eff} for both V & Ti
4.0	0.116	0.095
3.0	0.107	0.056
2.0	0.101	0.890

I1



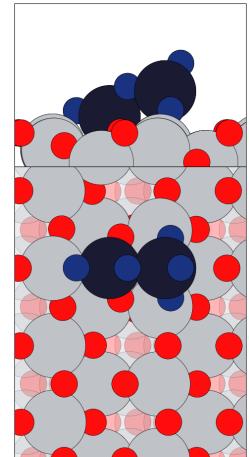
I2



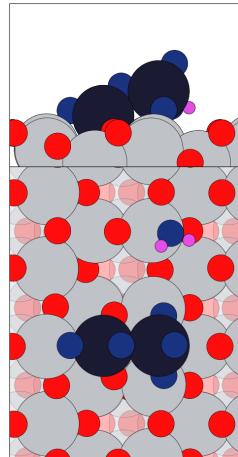
Adsorption Energies By addition of H₂O Molecule

E_1^{Ads}

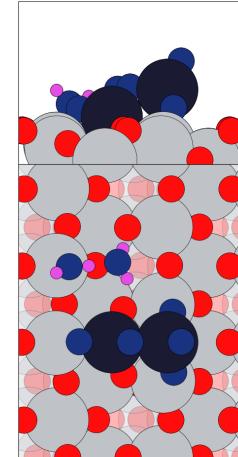
$$E_{\text{ads}} = E_{\text{tot.}}(n \text{ H}_2\text{O} + \text{V}_2\text{O}_5) / \text{a-TiO}_2(101) - n E_{\text{tot}}(\text{H}_2\text{O}) - E_{\text{tot}}((\text{VO})_x + \text{a-TiO}_2(101))$$



$\Delta E = 0.000 \text{ eV}$



$\Delta E = 0.076 \text{ eV}$

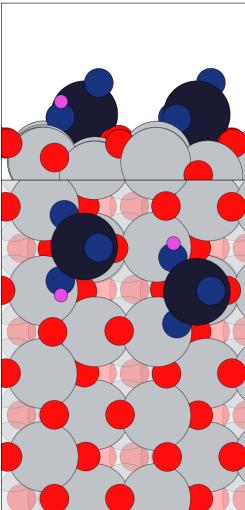


$\Delta E = 0.271 \text{ eV}$

	$E_{\text{ads}}(1 \text{ H}_2\text{O}) \text{ (eV)}$	$E_{\text{ads}}(2 \text{ H}_2\text{O}) \text{ (eV)}$	$E_{\text{ads}}(3 \text{ H}_2\text{O}) \text{ (eV)}$	$E_{\text{ads}}(5 \text{ H}_2\text{O}) \text{ (eV)}$
E_1^{Ads}	-0.871	1.546		
E_2^{Ads}	-1.264			
E_3^{Ads}	-1.013			
E_4^{Ads}	-0.912	-1.945	-2.929	-3.943
E_5^{Ads}	-1.982	-2.875	-3.694	-4.838

E_2^{Ads}

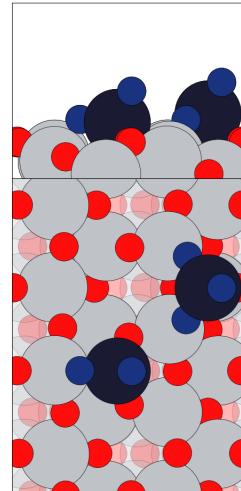
$H_2\text{O} \rightarrow$



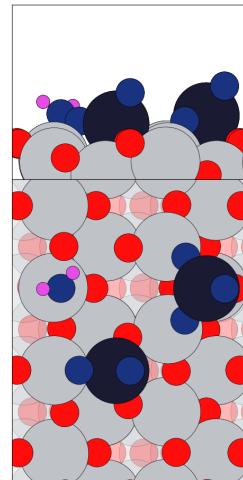
$\Delta E = 0.000 \text{ eV}$

E_3^{Ads}

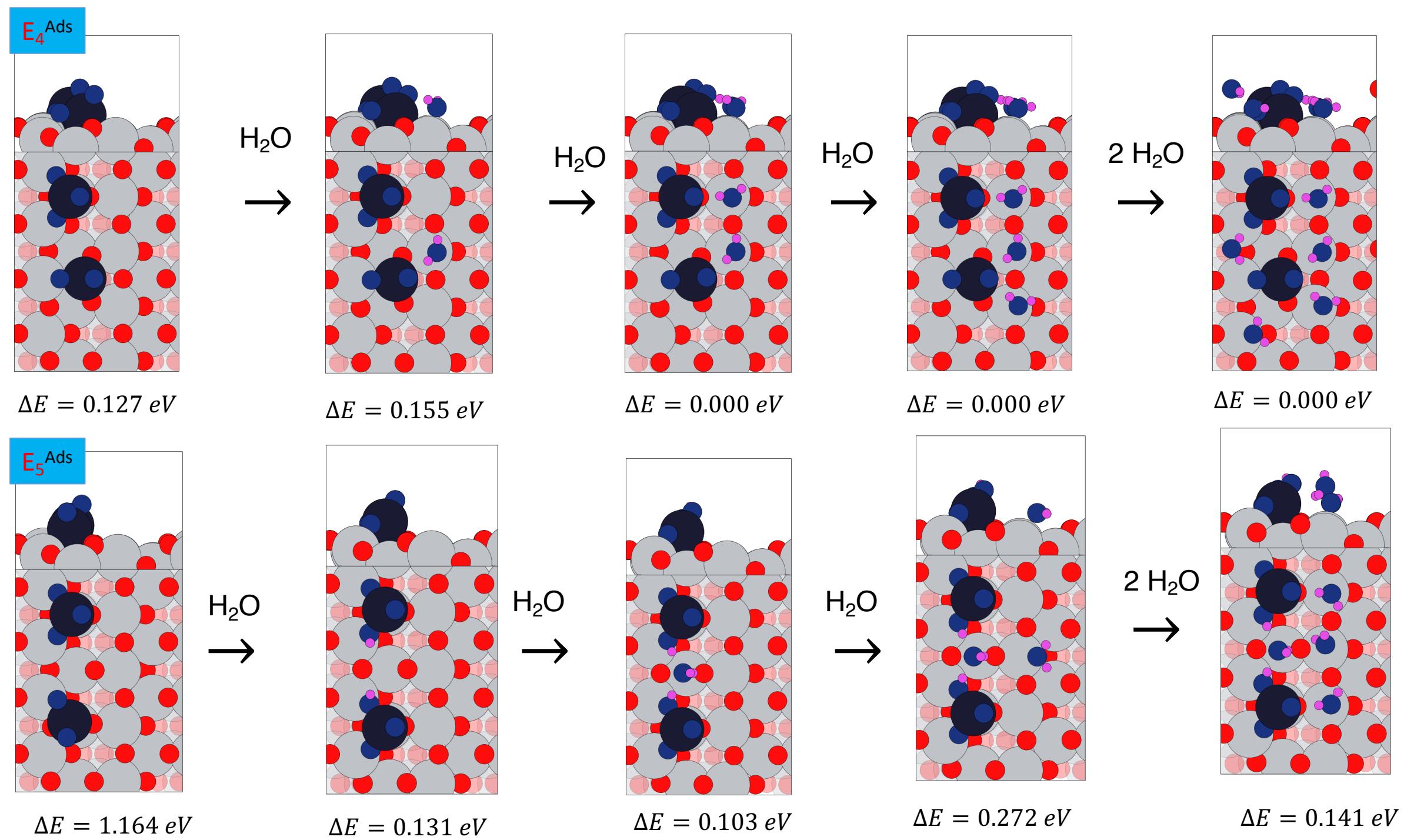
$H_2\text{O} \rightarrow$



$\Delta E = 0.131 \text{ eV}$



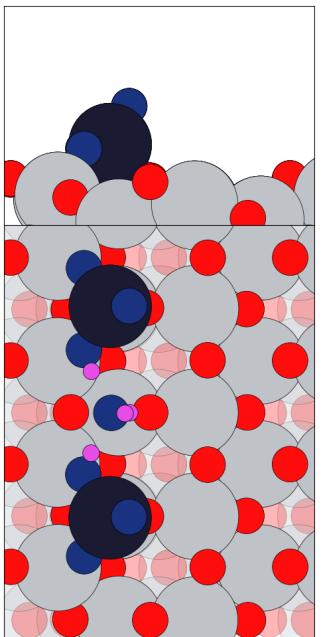
$\Delta E = 0.066 \text{ eV}$



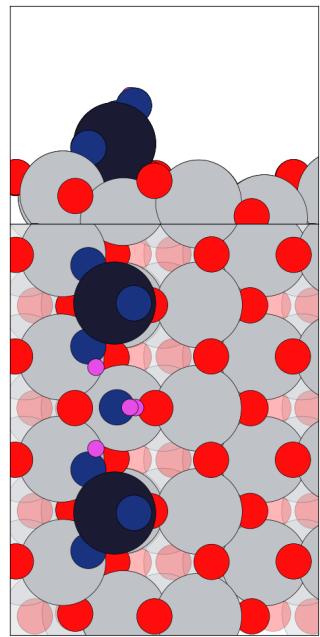
Observations

1) Effect of O-vacancy:

There is gain in energy due to O-vacancy in the subcell surface. The gain in energy is around in the range of 0.05 eV to 0.200 eV depends upon the structure. Due to this there is change in the order of low-lying isomers which are in the range of meV.



O-vacancy
→



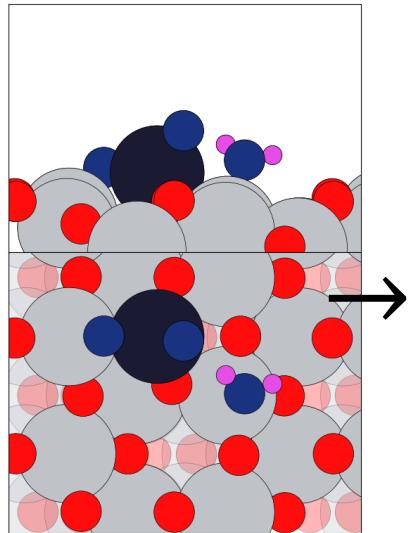
I4: $\Delta E = 0.254 \text{ eV}$

I2: $\Delta E = 0.103 \text{ eV}$

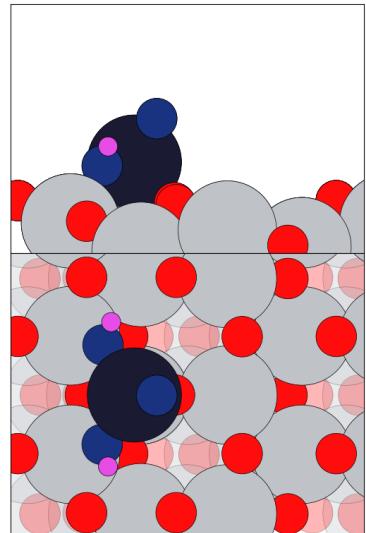
Observations

2) Dissociation capability of H₂O due to size of Cluster:

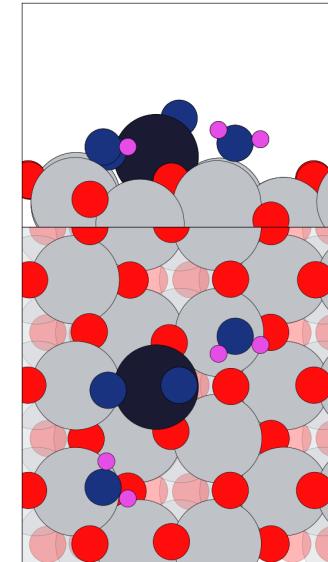
In case of VO₂ cluster, it requires 0.131 eV/1 H₂O and 0.053 eV/2 H₂O energy to dissociate the H₂O. And In case of V₂O₄ and V₂O₅, dissociated H₂O strcture is the GM.



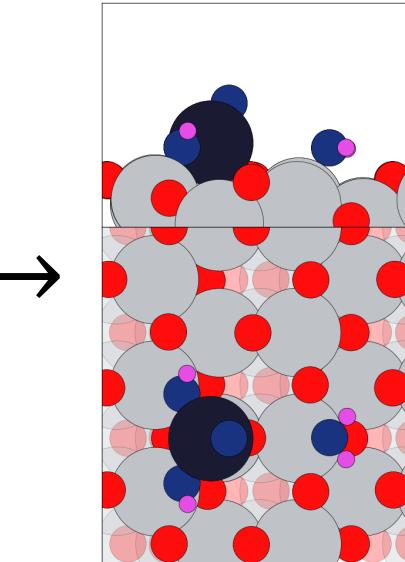
I1: $\Delta E = 0.000 \text{ eV}$



I2: $\Delta E = 0.131 \text{ eV}$



I1: $\Delta E = 0.000 \text{ eV}$

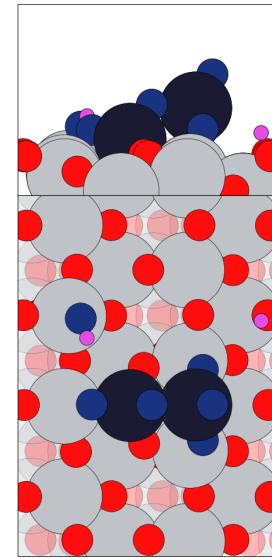
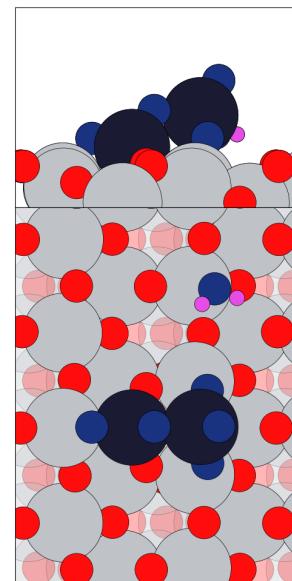
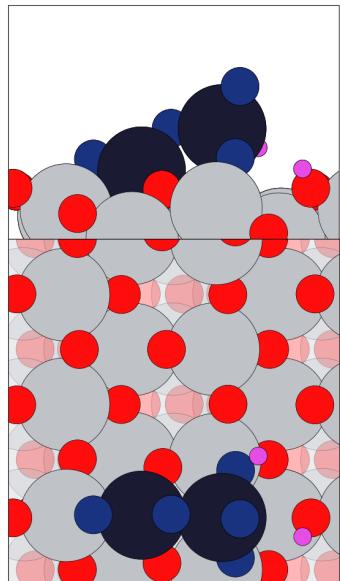
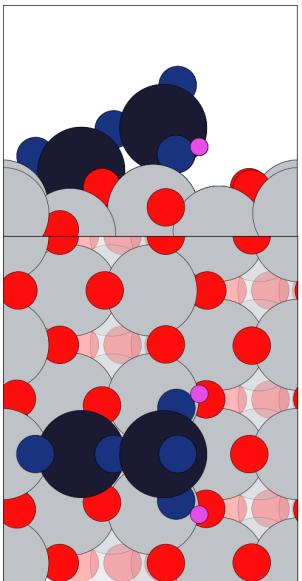


I3: $\Delta E = 0.053 \text{ eV}$

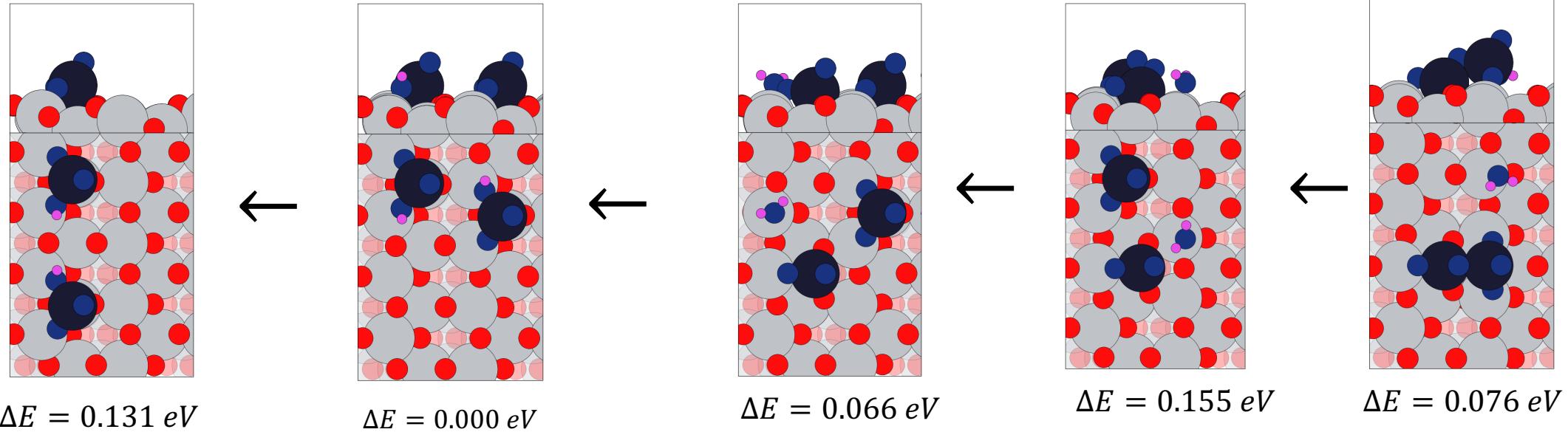
Observations

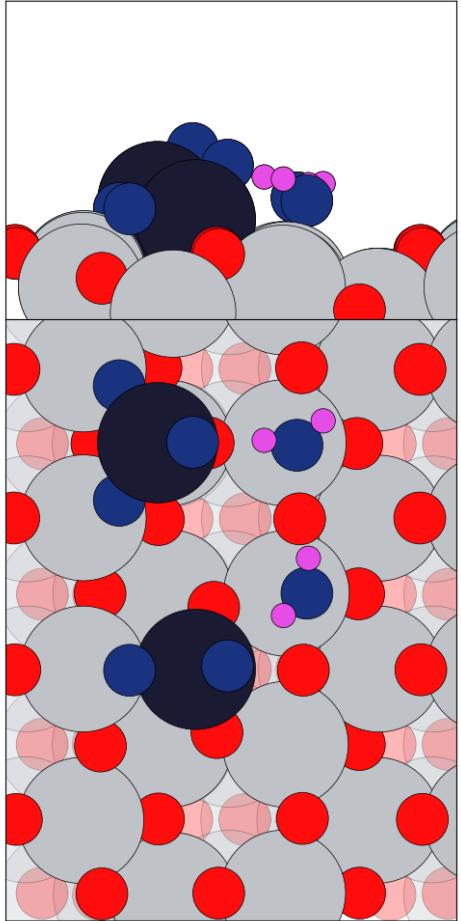
3) Surface Effect on H₂O dissociation:

We did not observed the surface hydroxyls within 0.2 eV energy range from GM. Mostly Vanadium oxide clusters are responsible for H₂O dissociation.

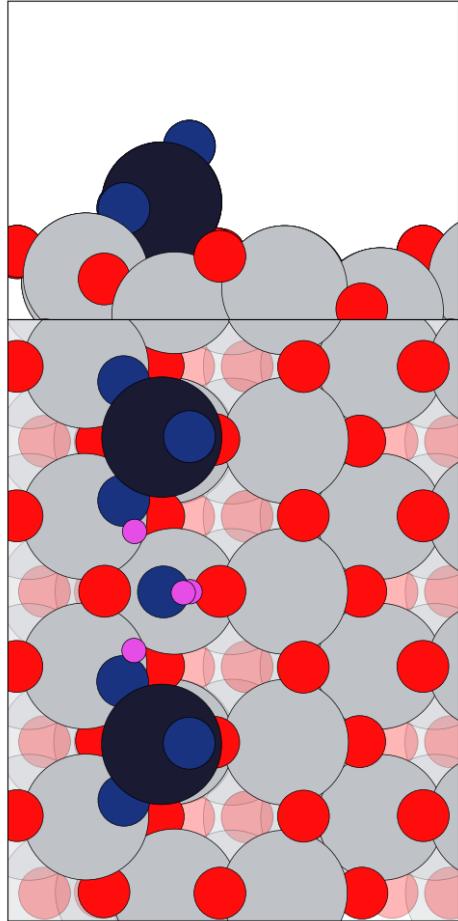


Adsorption Energy order

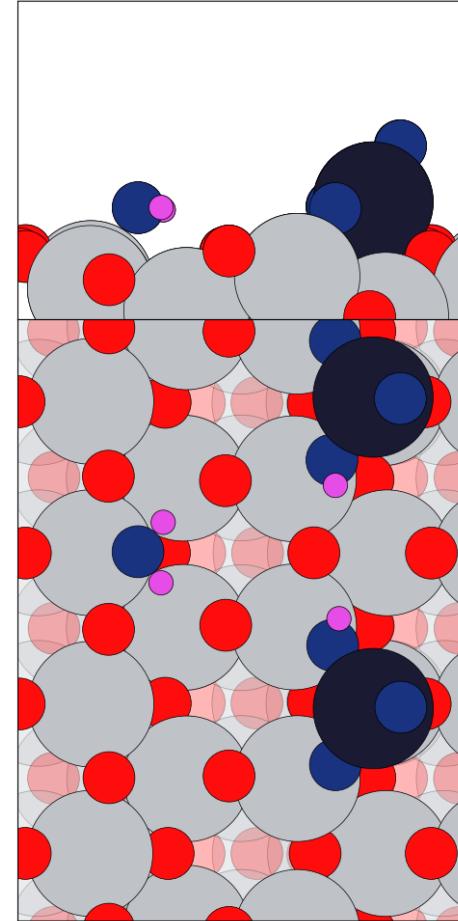




$$\Delta E = 0.000 \text{ eV}$$

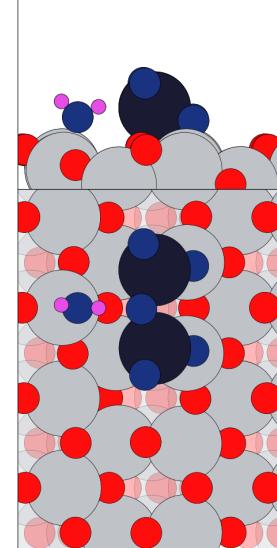
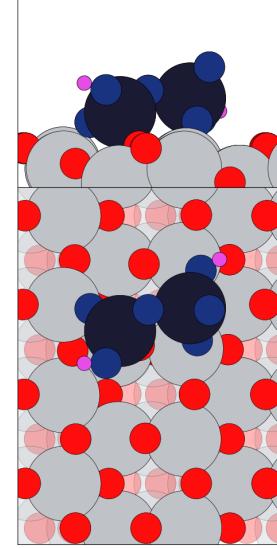
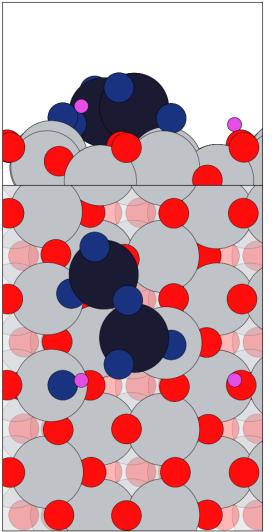
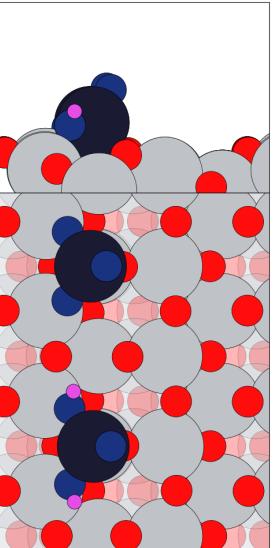
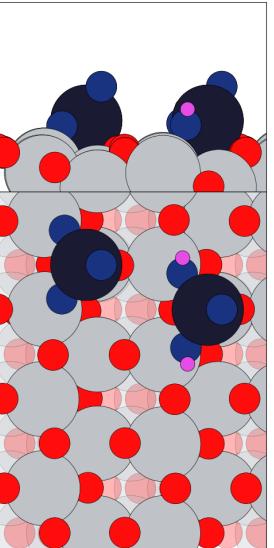
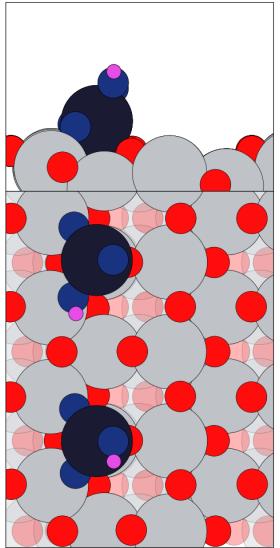


$$\Delta E = 0.08 \text{ eV}$$



$$\Delta E = 0.150 \text{ eV}$$

Binding Energy of H₂O for V₂O₅+H₂O (O_v+csr)



I9:E_{bind} = -0.767 eV

I10:E_{bind} = -0.717 eV

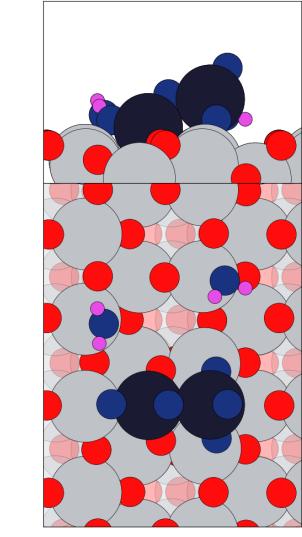
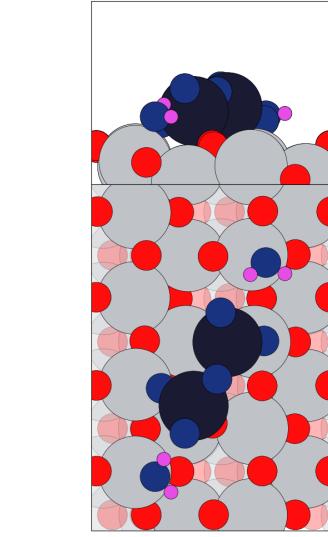
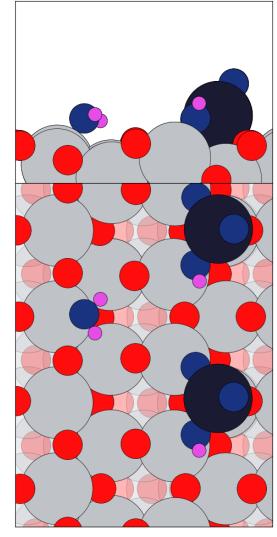
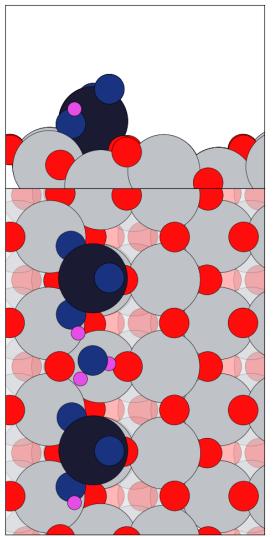
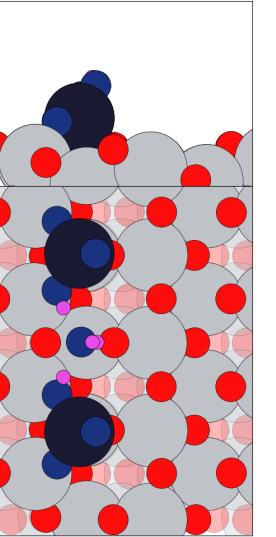
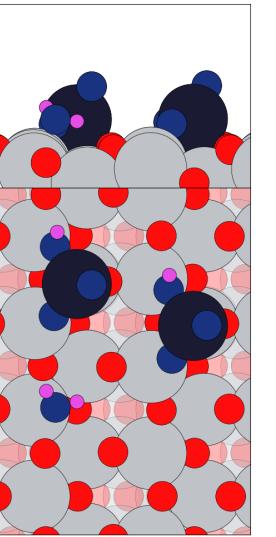
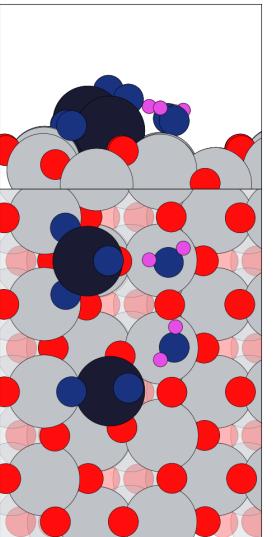
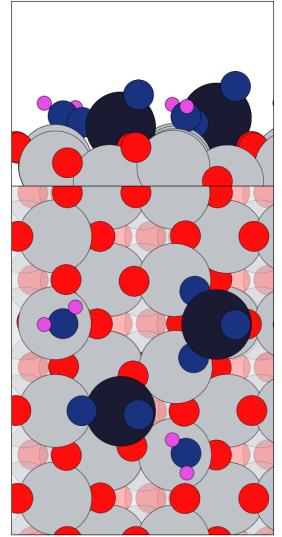
I11:E_{bind} = -0.609 eV

I12:E_{bind} = -0.550 eV

I13:E_{bind} = -0.465 eV

I14:E_{bind} = -0.428 eV

Binding Energy of H₂O for V₂O₅+2 H₂O (O_v+csr)



I1:E_{bind} = -1.864 eV

I1:E_{bind} = -1.816 eV

I1:E_{bind} = -1.809 eV

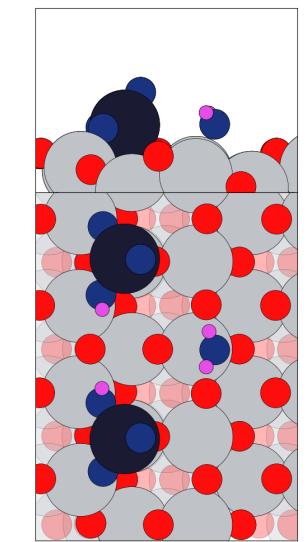
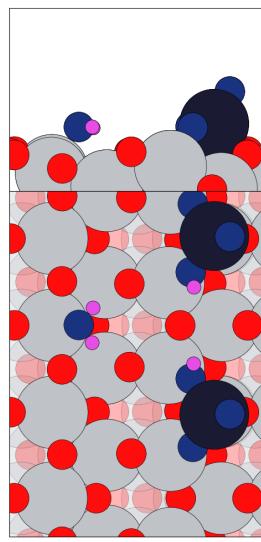
I2:E_{bind} = -1.710 eV

I3:E_{bind} = -1.698 eV

I3:E_{bind} = -1.693 eV

I4:E_{bind} = -1.646 eV

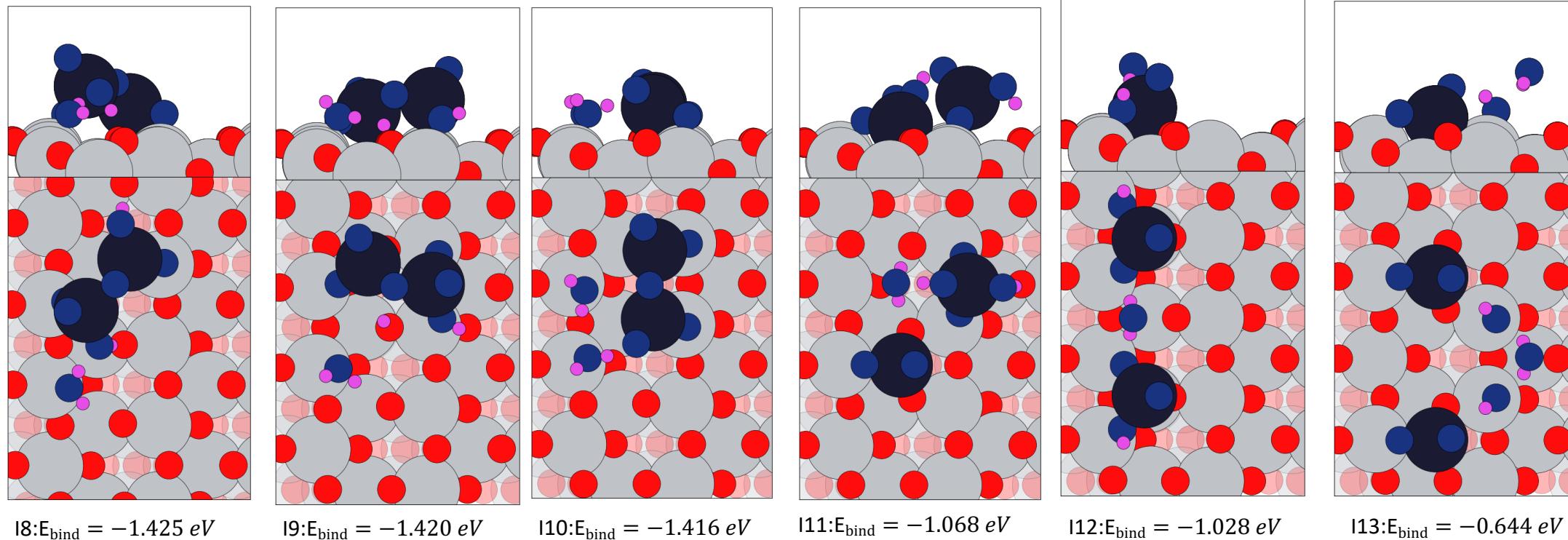
I6:E_{bind} = -1.637 eV

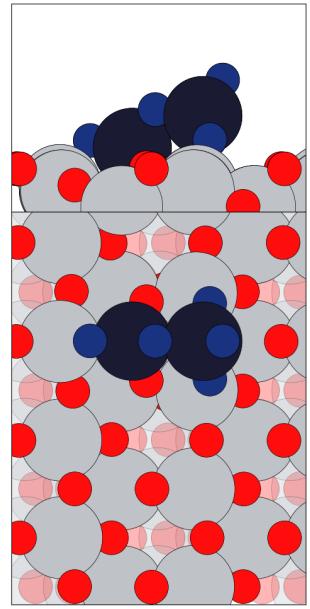


I5:E_{bind} = -1.632 eV

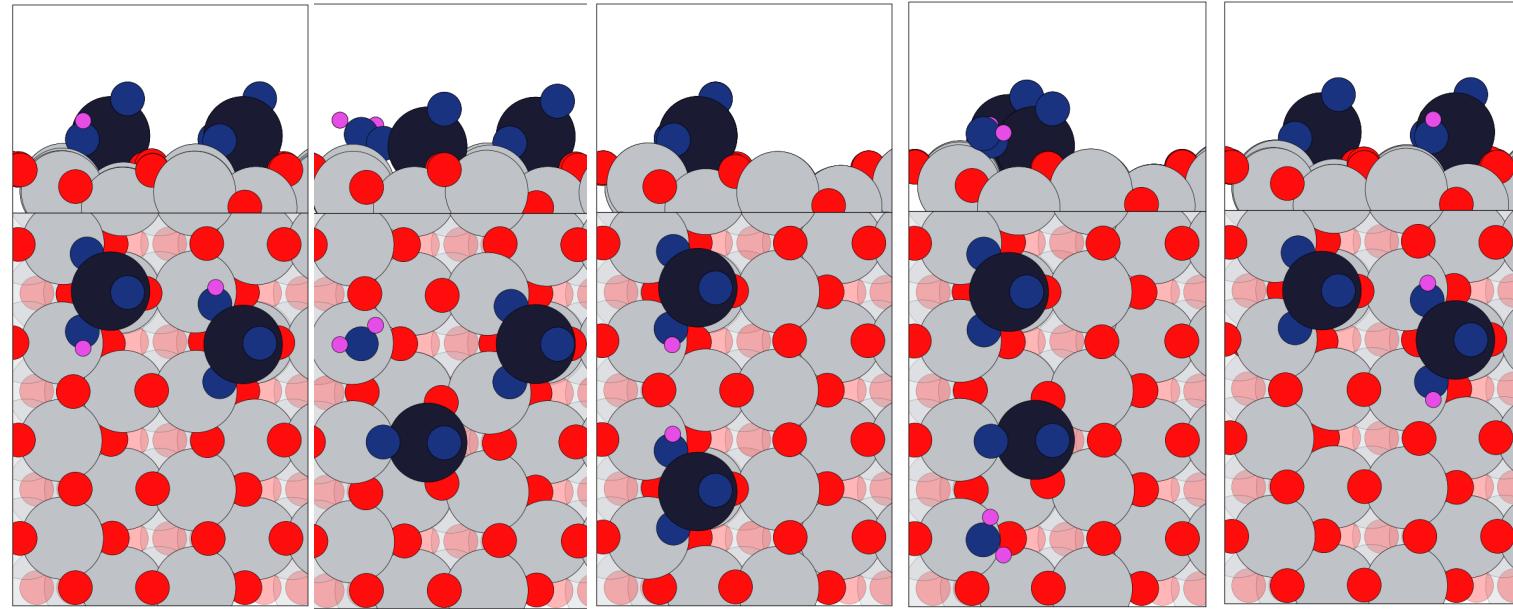
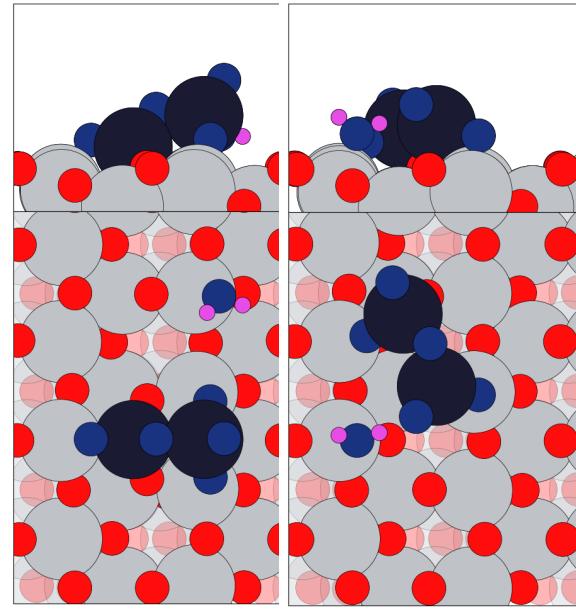
I7:E_{bind} = -1.438 eV

Binding Energy of H₂O for V₂O₅+2 H₂O (O_v+csr)

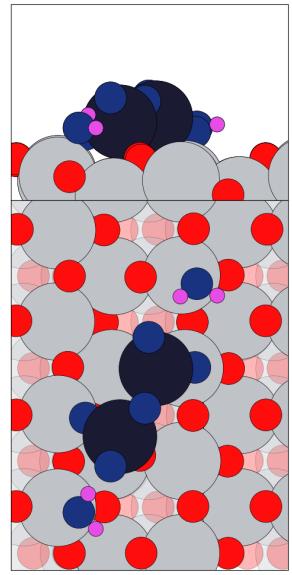




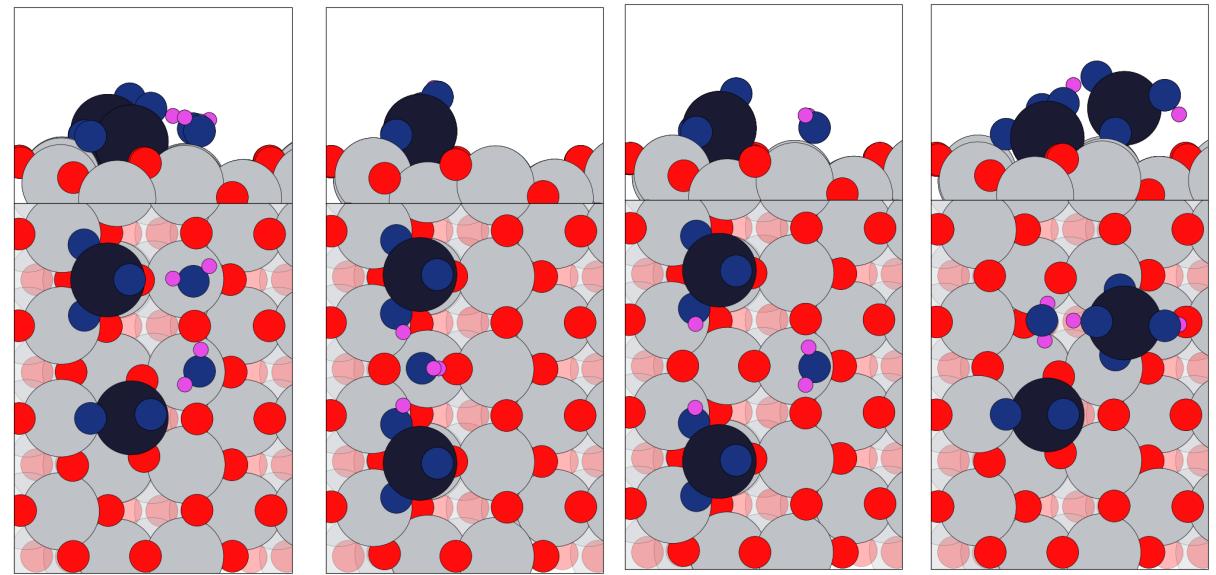
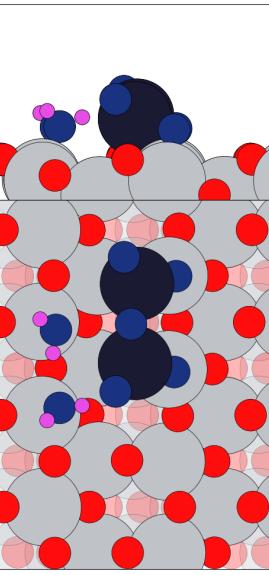
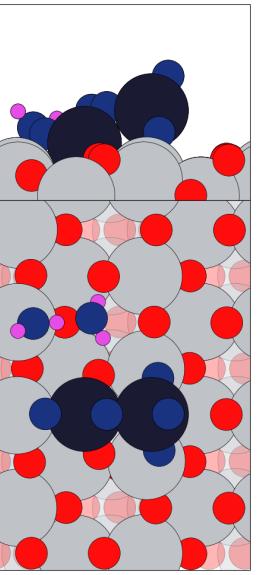
I3: $E_{\text{bind}} = -0.871 \text{ eV}$ I7: $E_{\text{bind}} = -0.780 \text{ eV}$



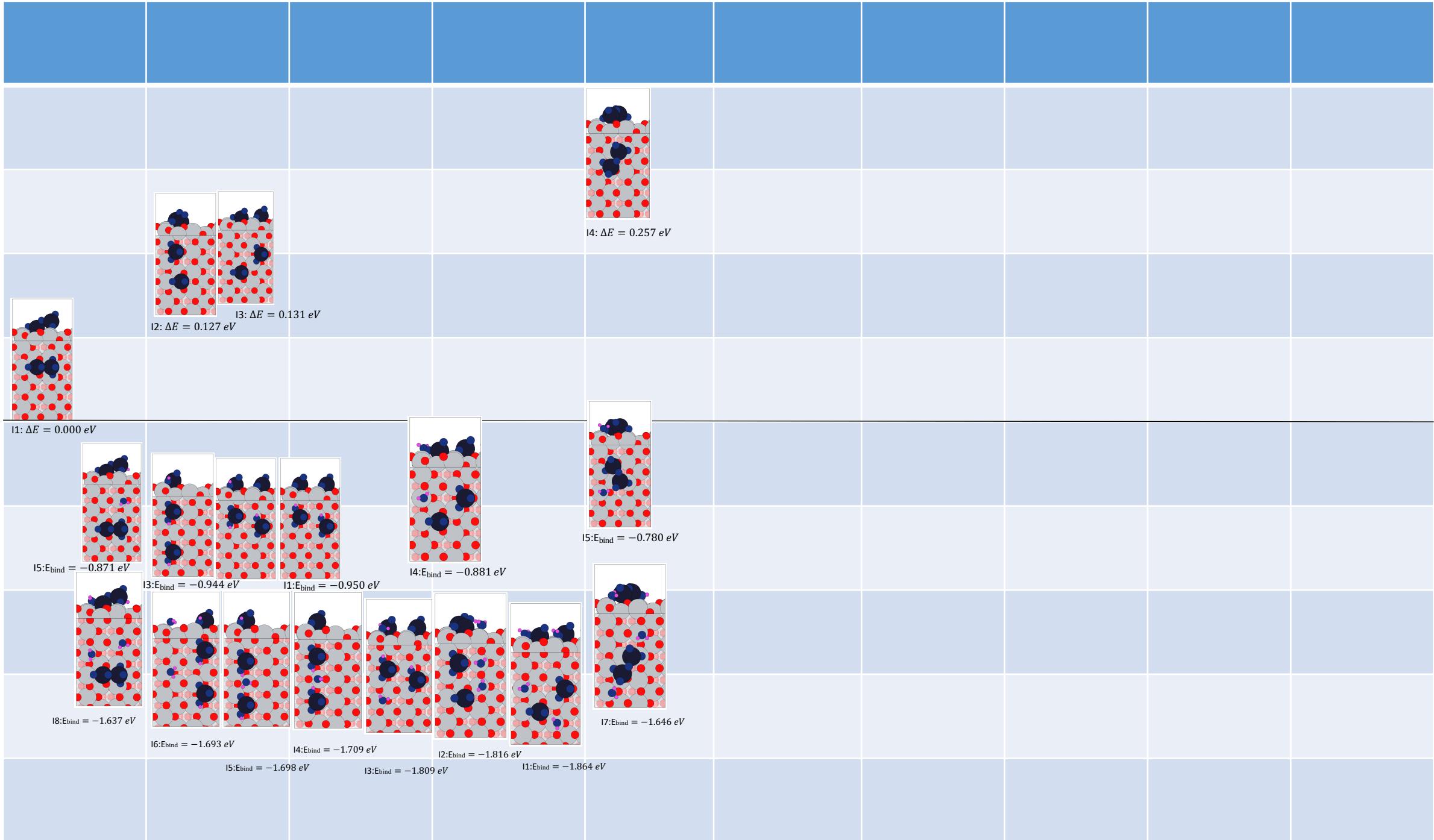
I1: $E_{\text{bind}} = -0.948 \text{ eV}$ I2: $E_{\text{bind}} = -0.881 \text{ eV}$ I5: $E_{\text{bind}} = -0.816 \text{ eV}$ I8: $E_{\text{bind}} = -0.751 \text{ eV}$ I9: $E_{\text{bind}} = -0.717 \text{ eV}$



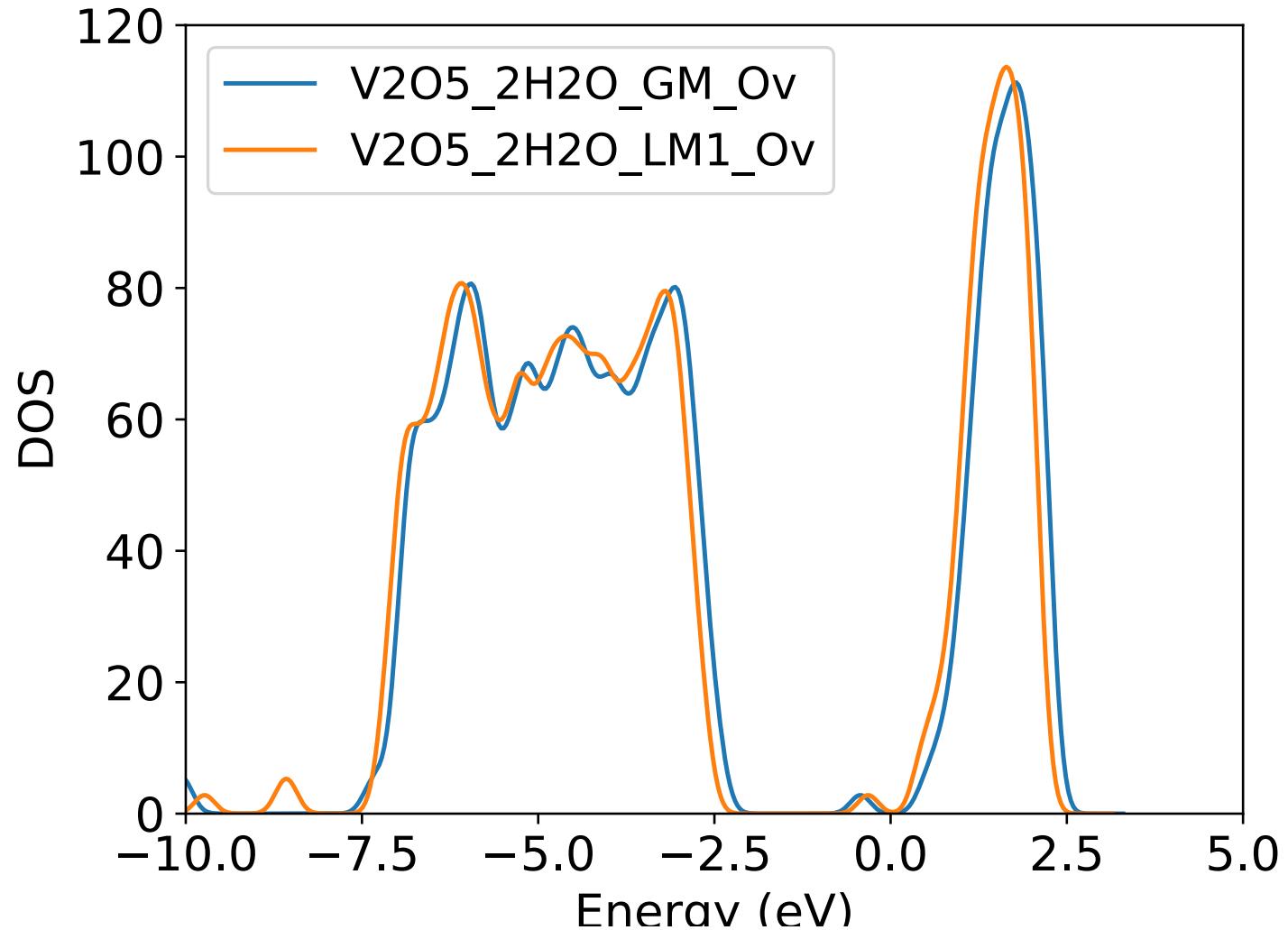
I3: $E_{\text{bind}} = -0.823 \text{ eV}$ I4: $E_{\text{bind}} = -0.773 \text{ eV}$ I7: $E_{\text{bind}} = -0.708 \text{ eV}$



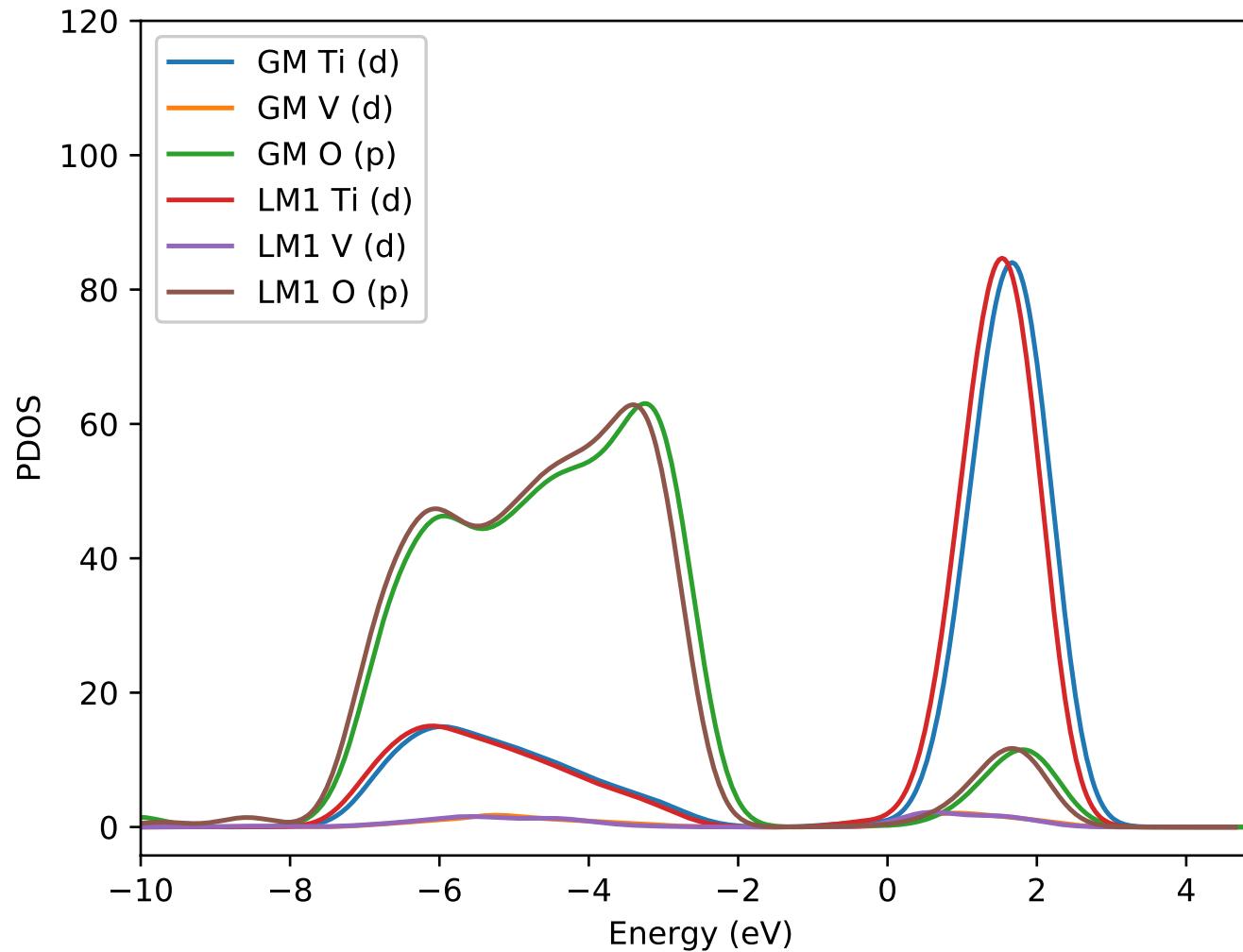
I1: $E_{\text{bind}} = -0.908 \text{ eV}$ I2: $E_{\text{bind}} = -0.855 \text{ eV}$ I5: $E_{\text{bind}} = -0.719 \text{ eV}$ I7: $E_{\text{bind}} = -0.534 \text{ eV}$

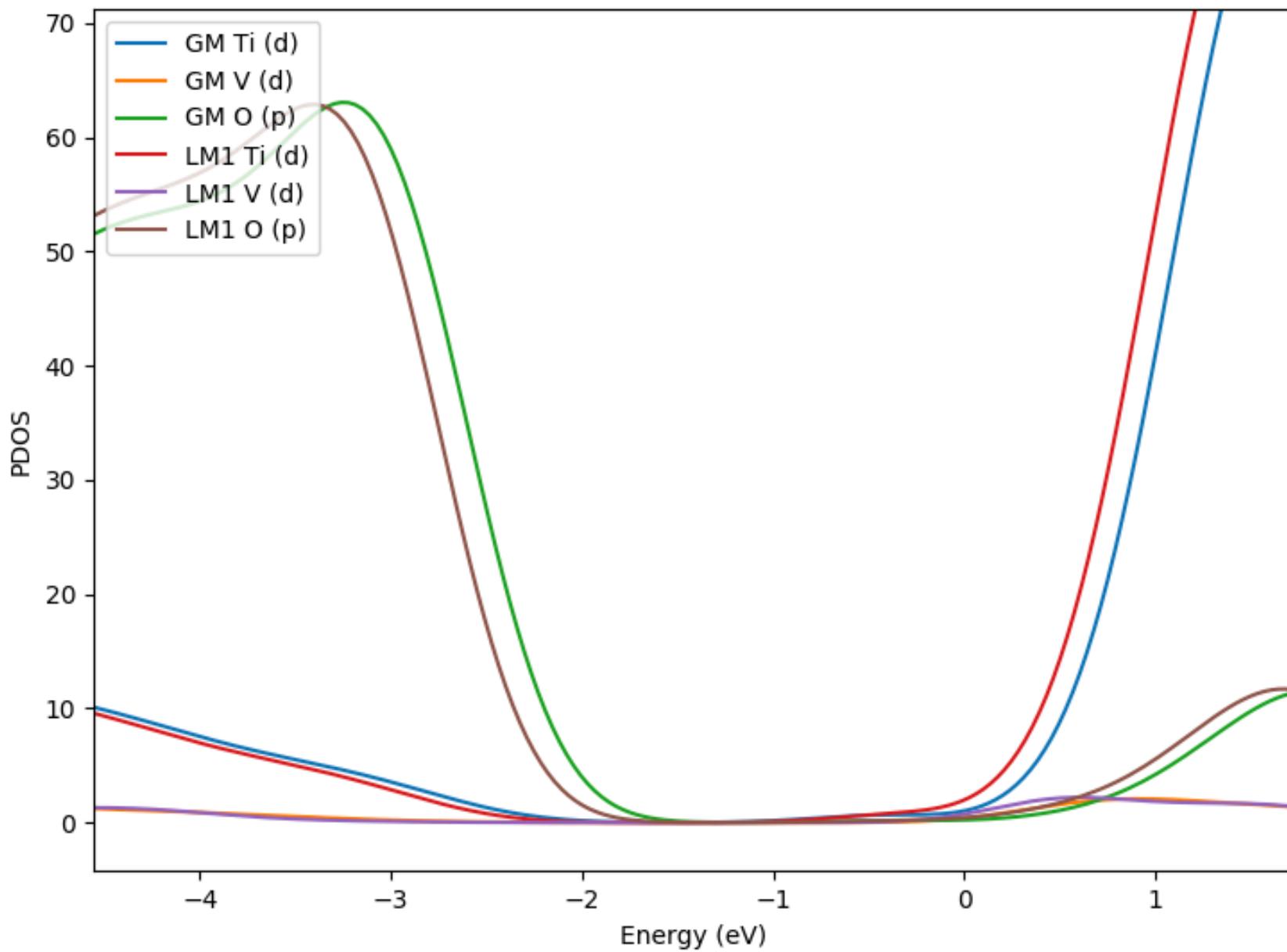


Density of States



Density of States





Observations

4) Dissociation of V₂O₅ clusters and Non-dissociation of V₂O₄ clusters:

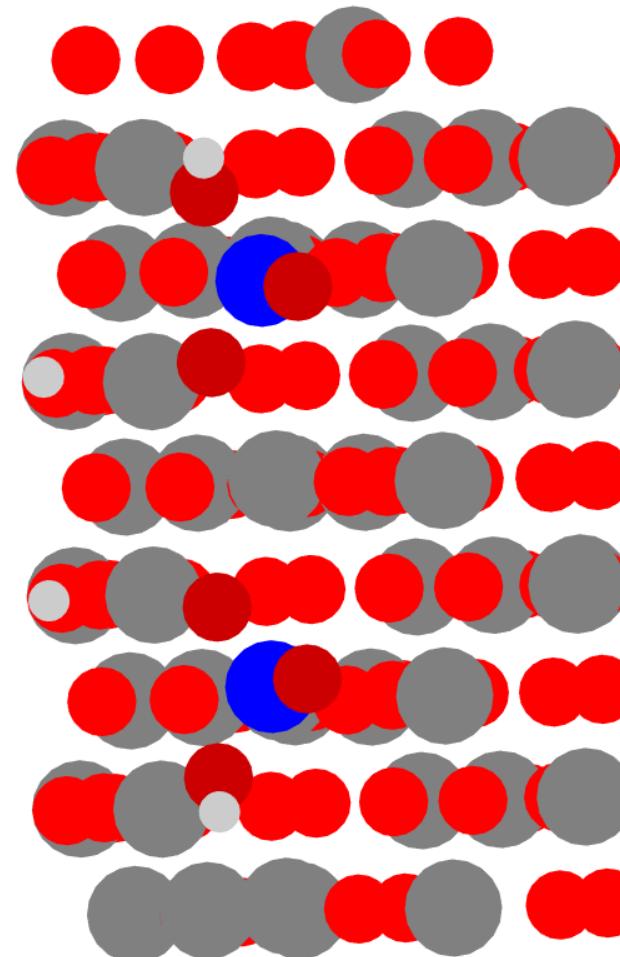
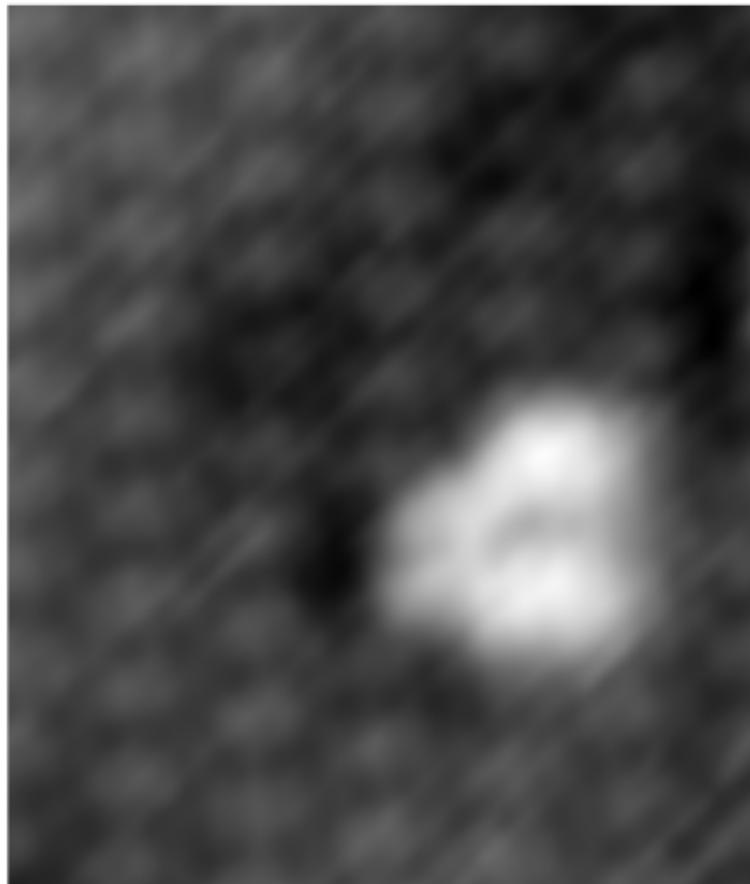
In case of V₂O₅ clusters during H₂O exposure, the cluster get dissociated in two paces (Ex: VO₃H) and in case of V₂O₄ during H₂O exposure also the clusters get remains intact due to keeping of +4 or +5 state of Vanadium oxidation state.

5) Restructuring of V₂O₅ cluster during H₂O exposure:

The re-structuring of V₂O₅ cluster during water exposure is due to dissociation of H₂O makes the V₂O₅ cluster in to two VO₃H clusters and these two VO₃H clusters can have different arrangements.

Suggestions for a structure

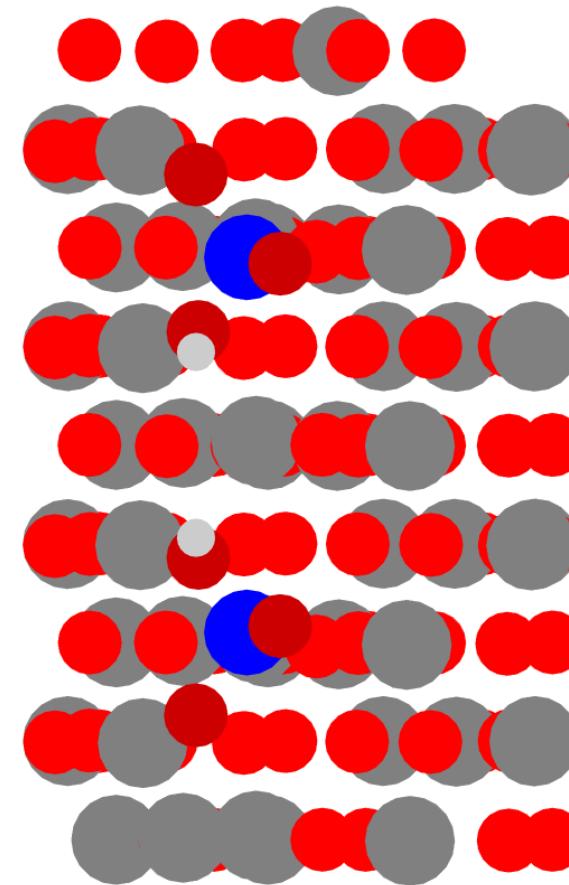
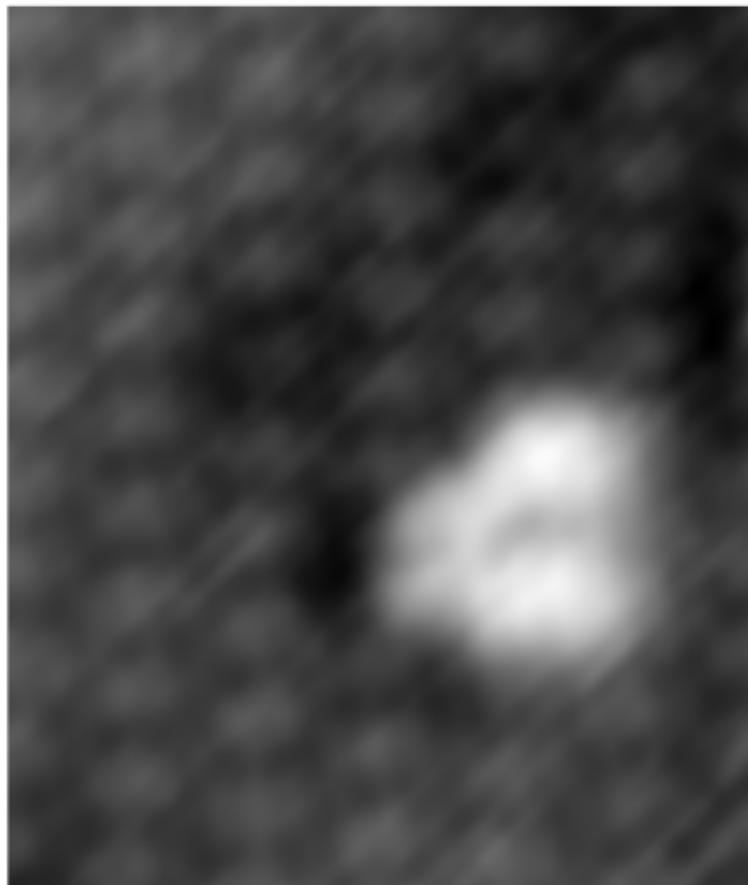
During Water exposure



2xV
6xO
4xH

Suggestions for a structure

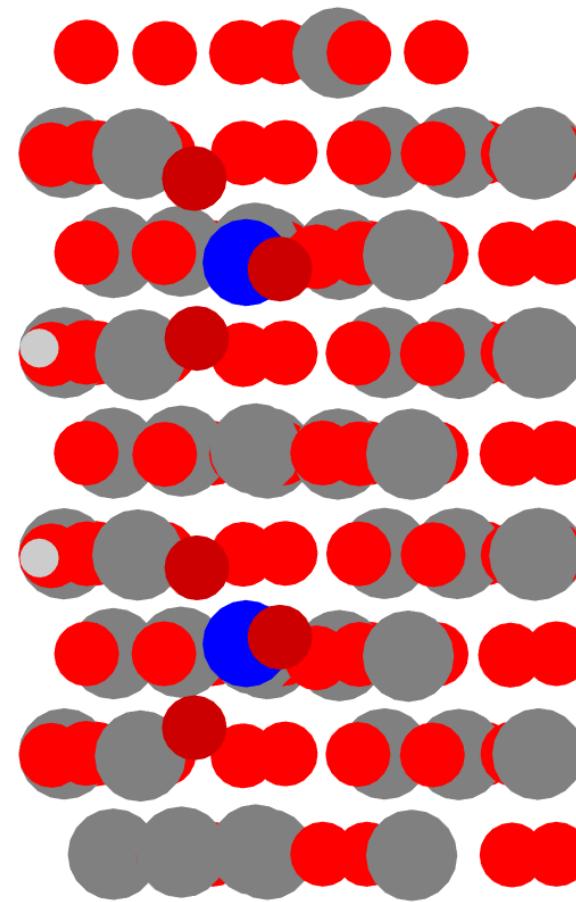
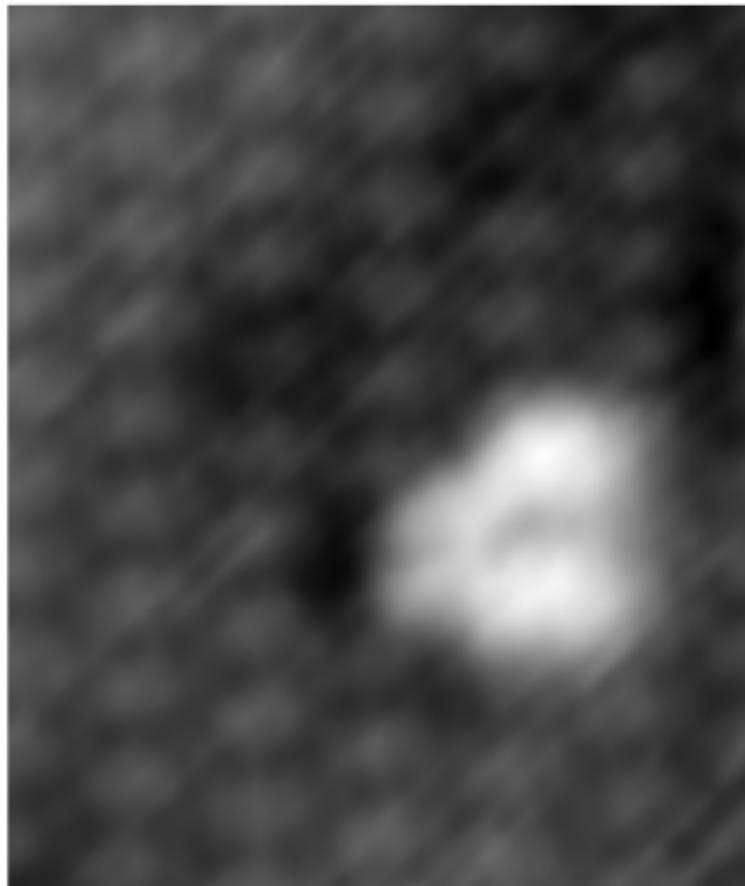
During Water exposure



2xV
6XO
2XH

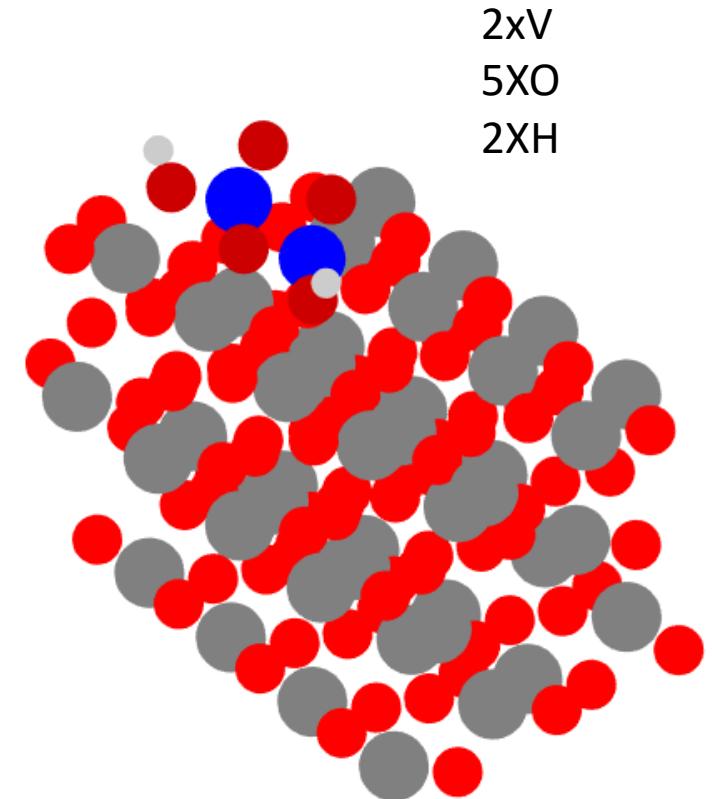
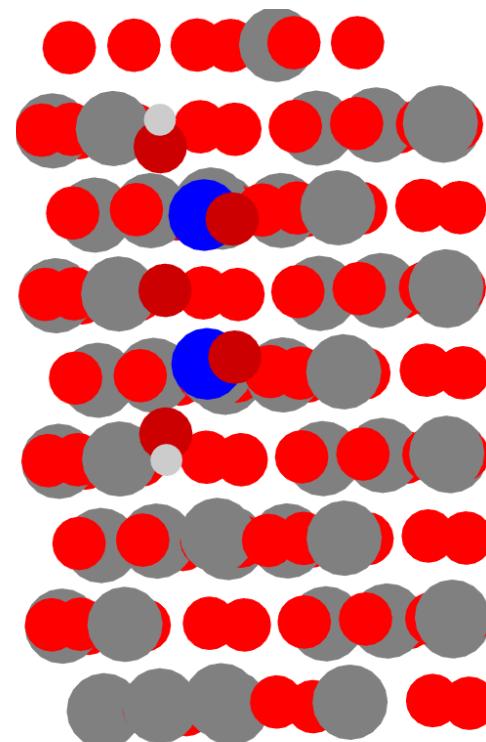
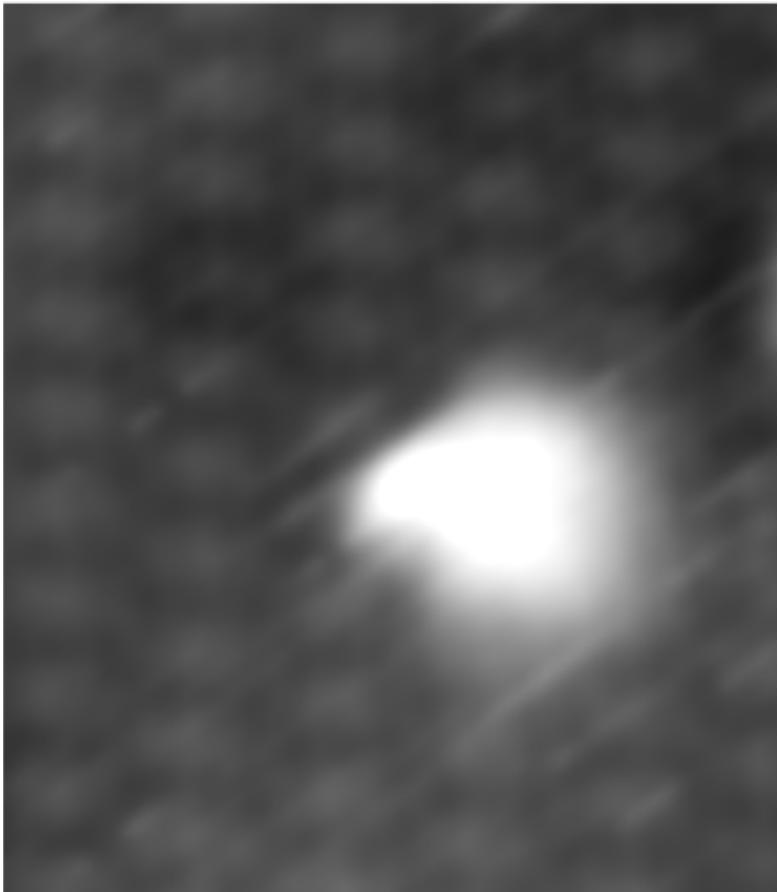
Suggestions for a structure

During Water exposure



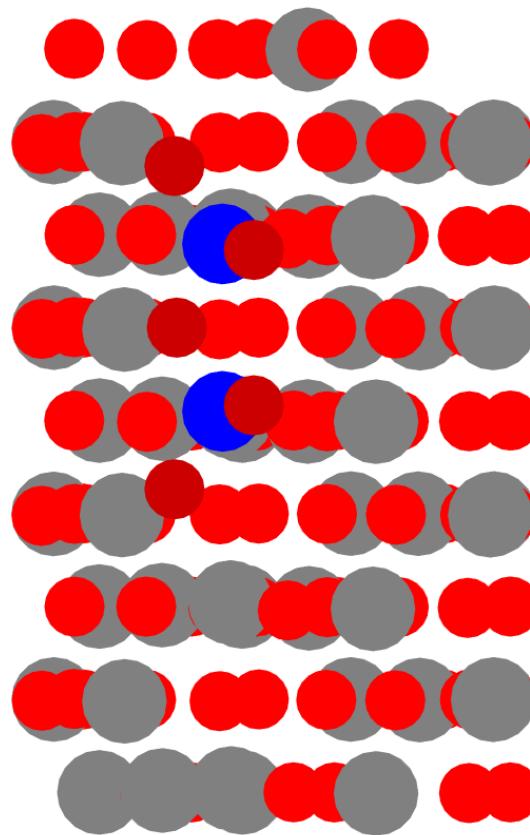
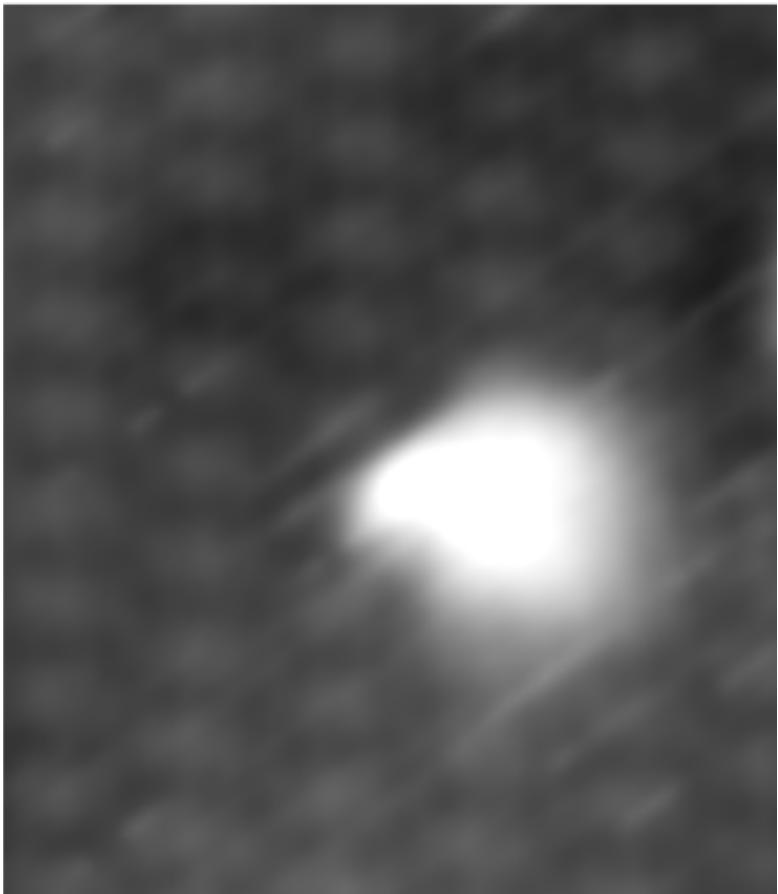
2xV
6XO
2XH

After Water Exposure



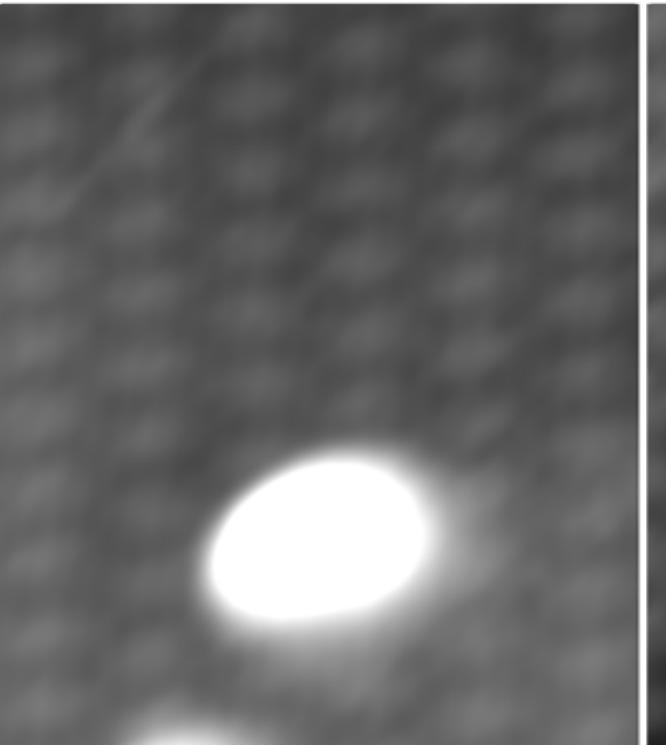
Placement of H is very
uncertain

After Water Exposure

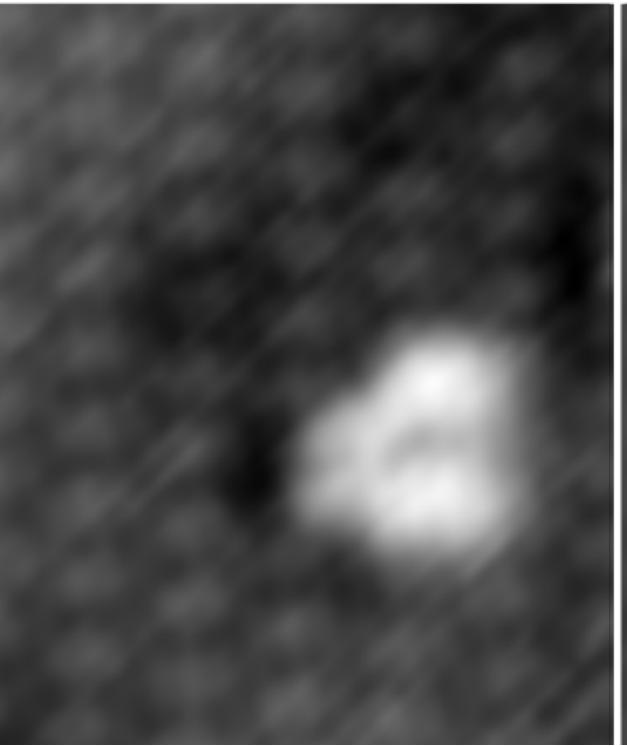


2xV
5XO

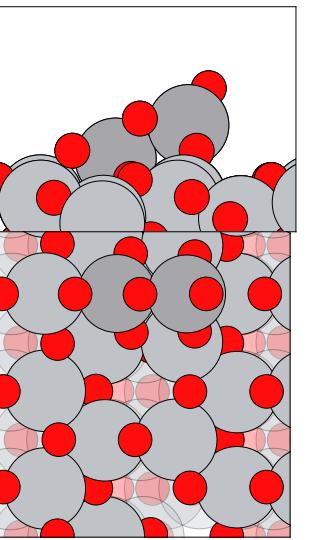
As-Deposited



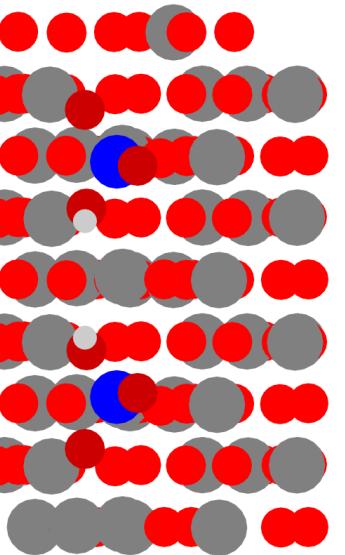
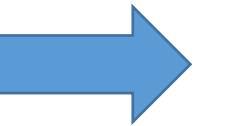
During Water exposure



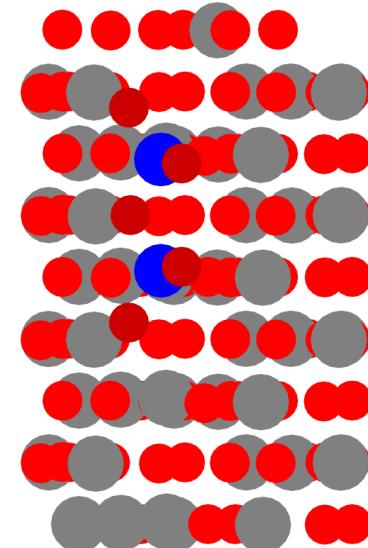
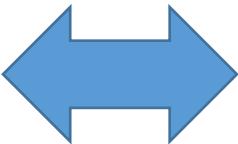
After Water Exposure



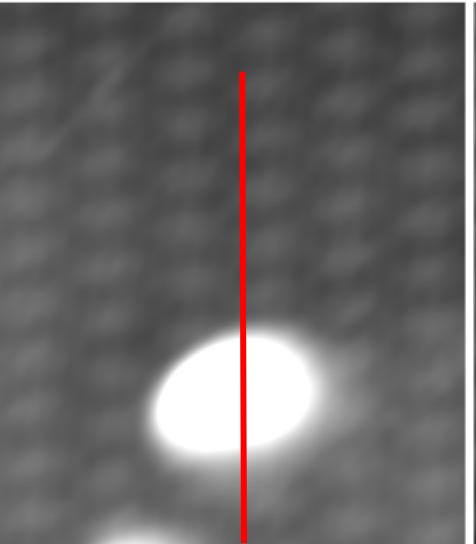
$1 \times H_2O$



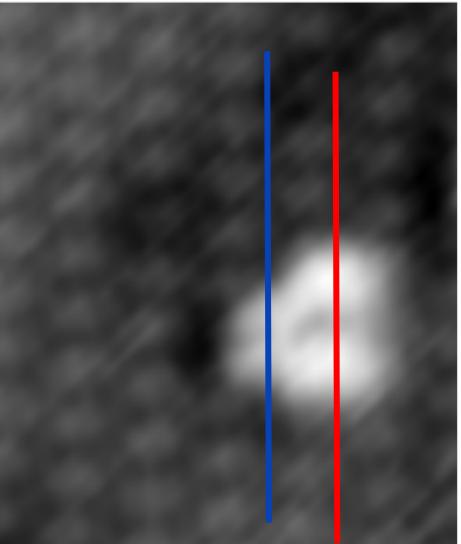
H_2O



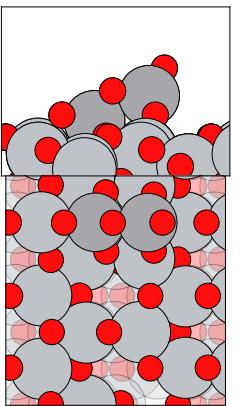
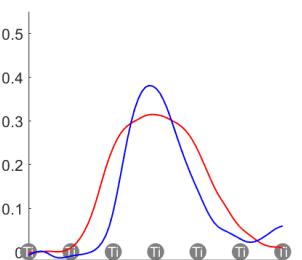
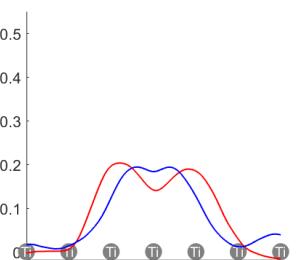
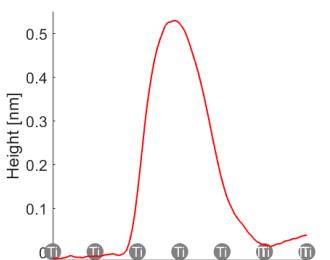
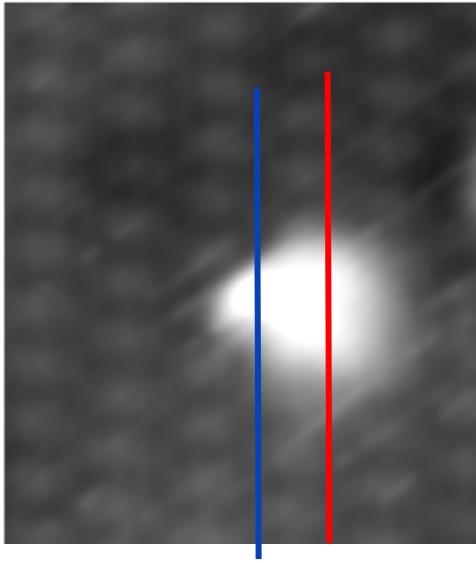
As-Deposited



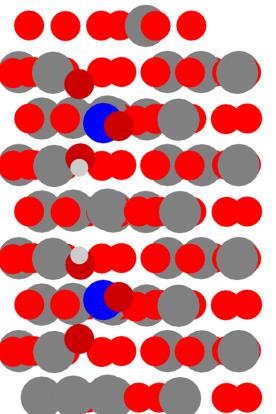
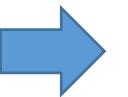
During Water exposure



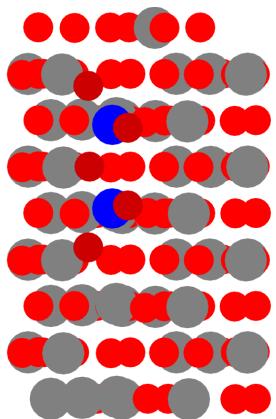
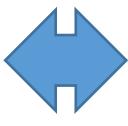
After Water Exposure



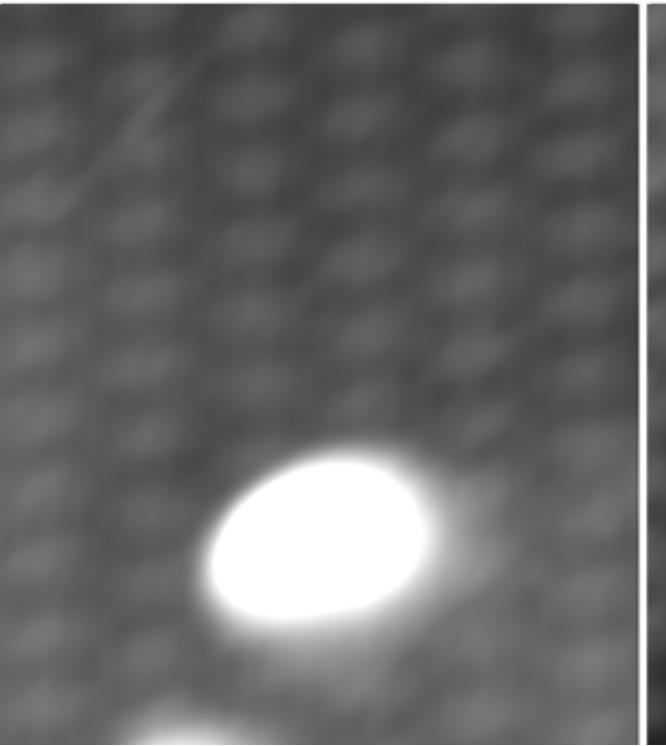
$1 \times H_2O$



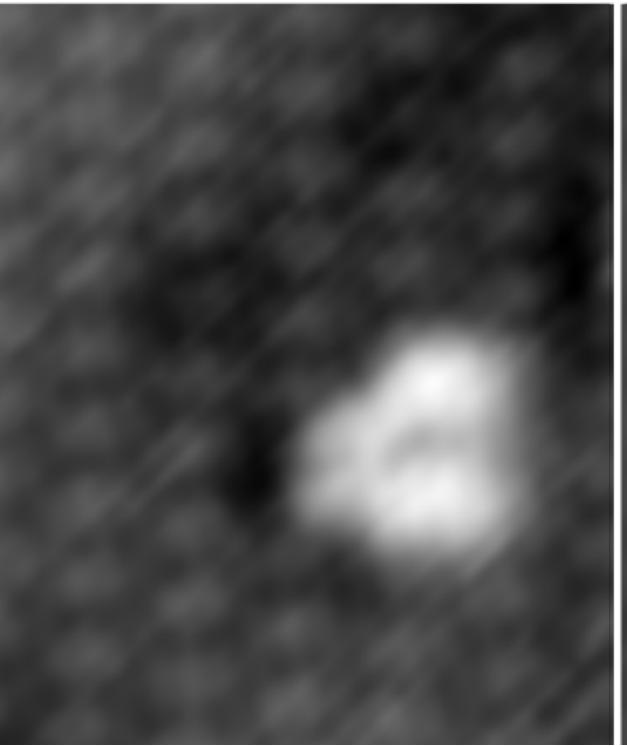
H_2O



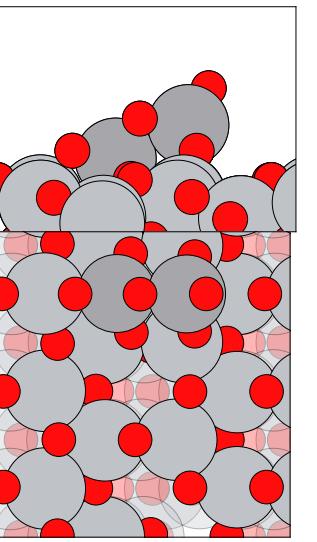
As-Deposited



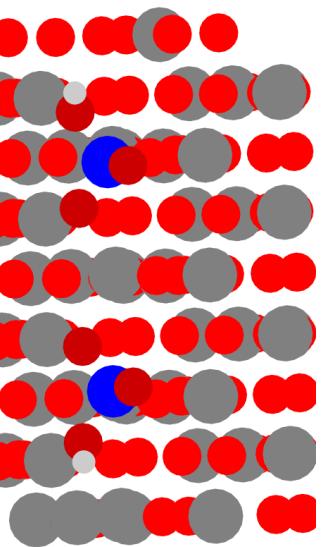
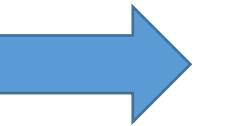
During Water exposure



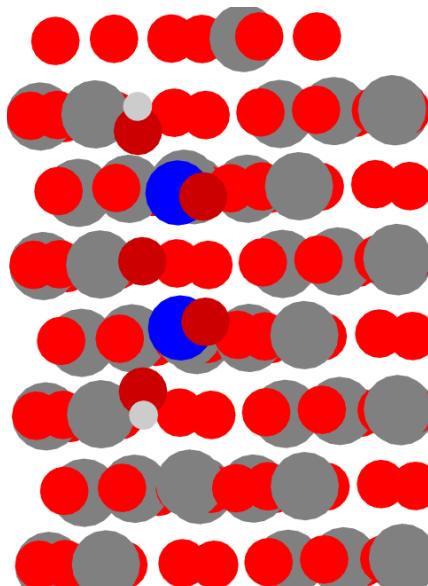
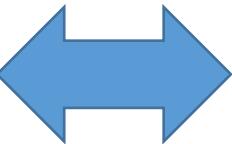
After Water Exposure



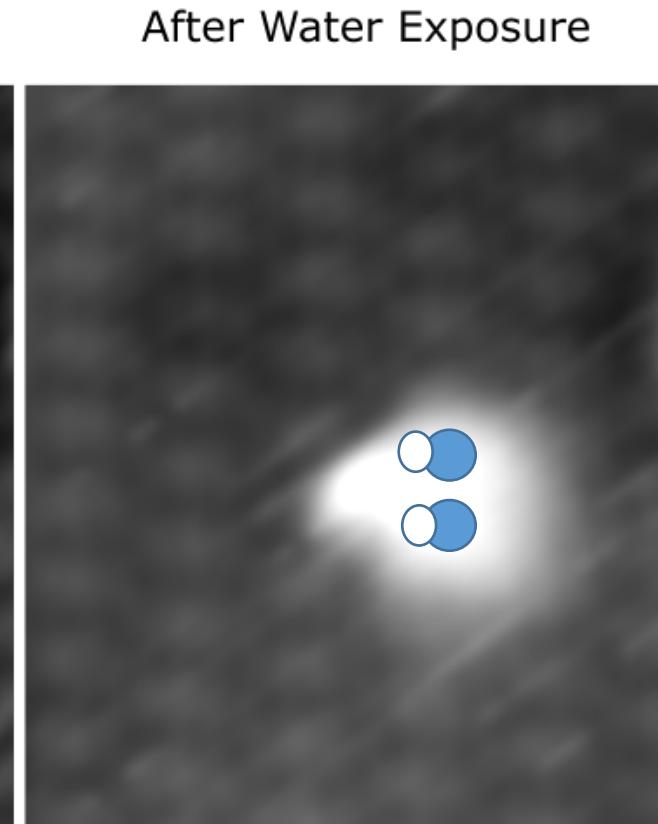
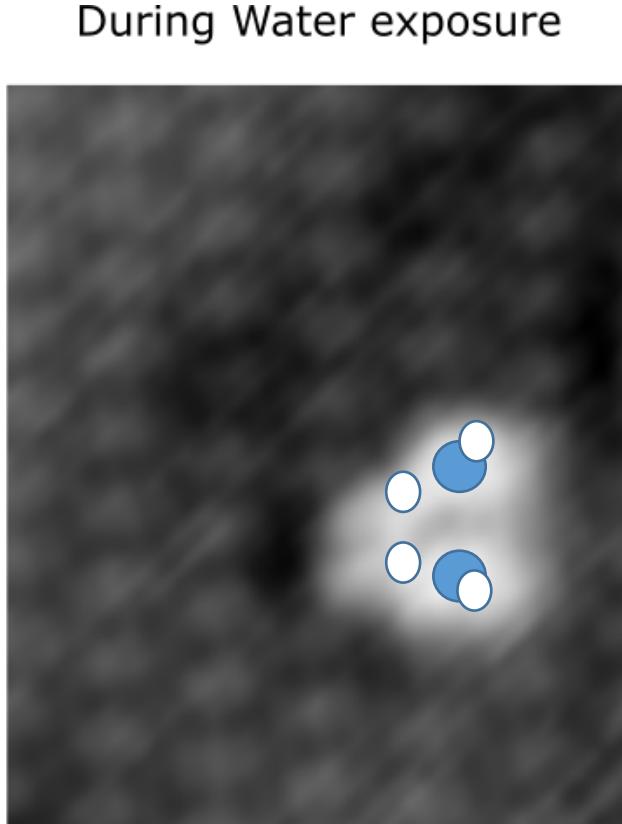
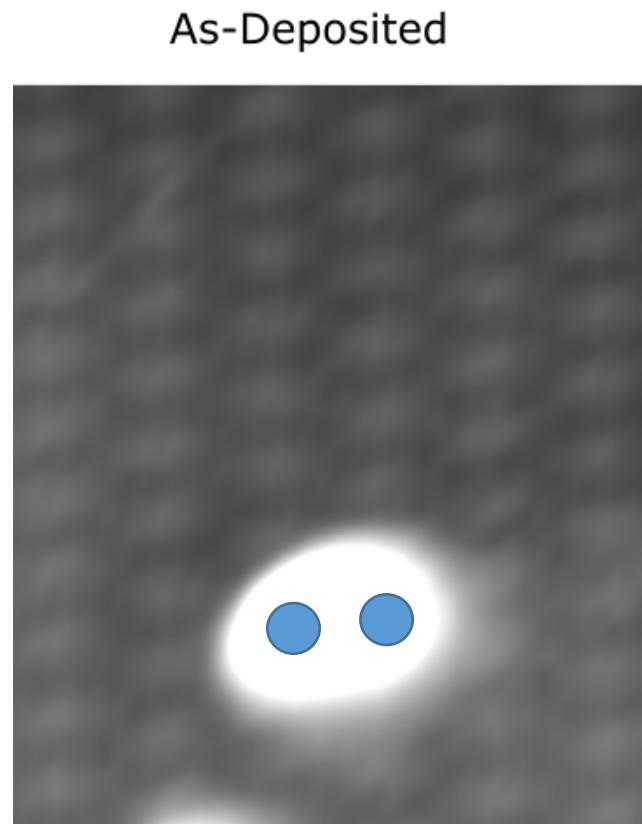
$1 \times H_2O$
 $2 \times H$



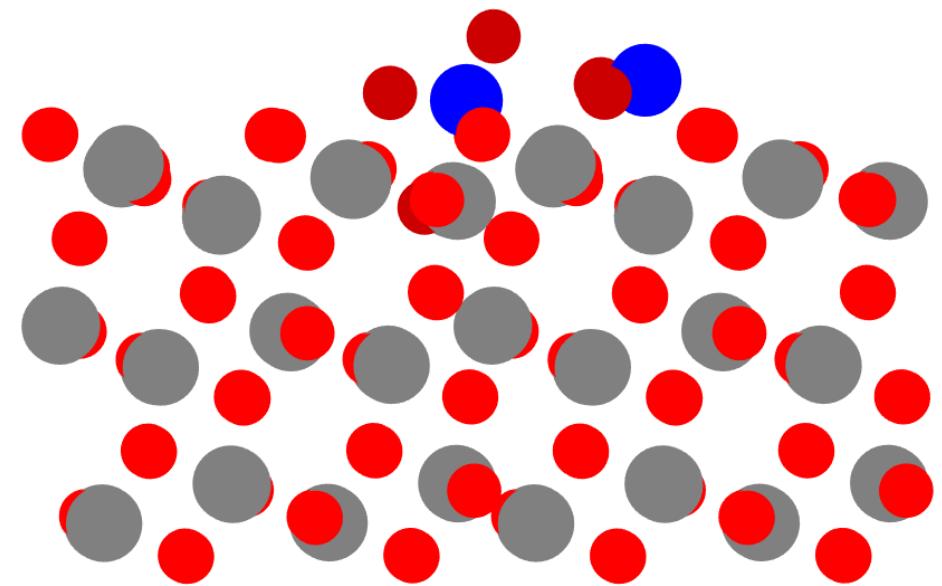
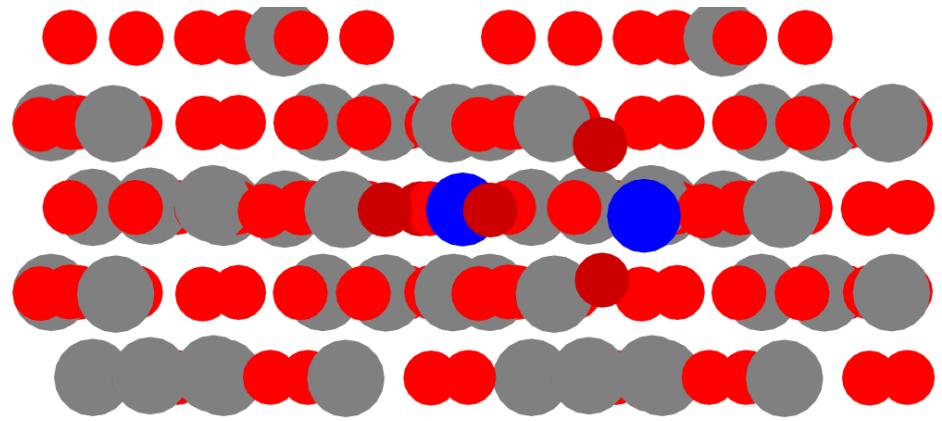
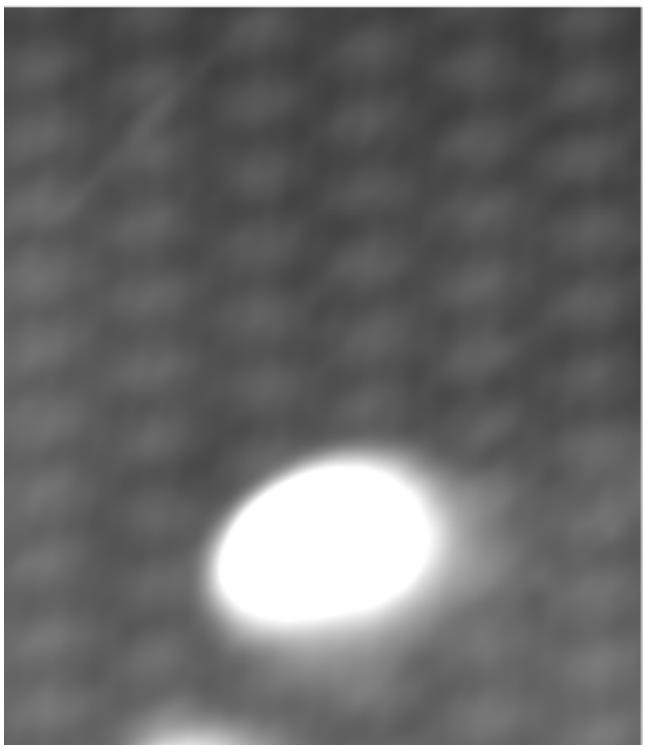
H_2O



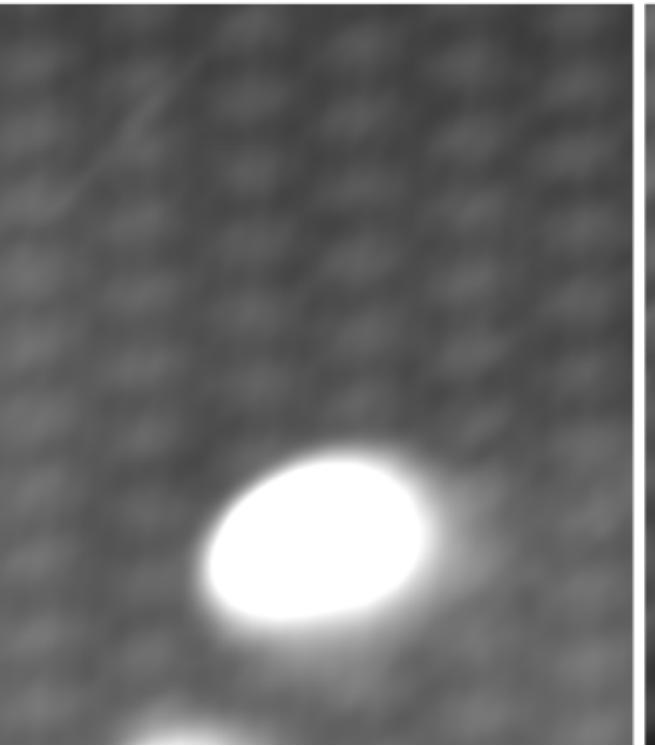
model suggestions



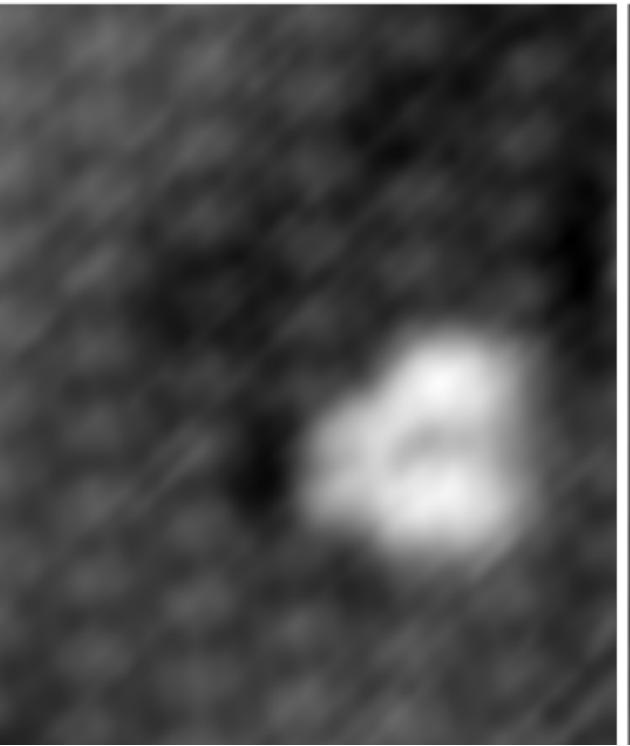
As-Deposited



As-Deposited



During Water exposure



After Water Exposure

