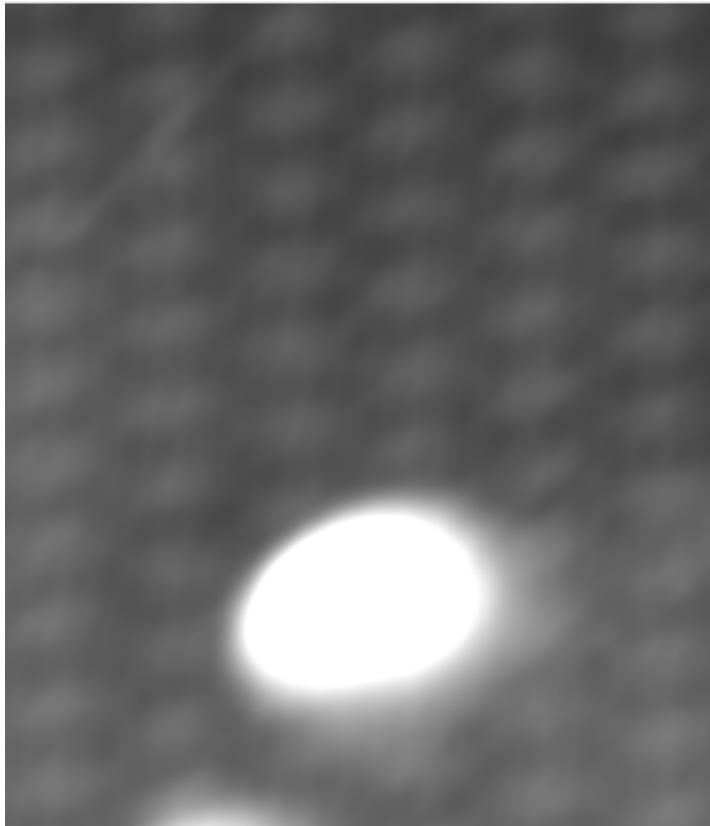
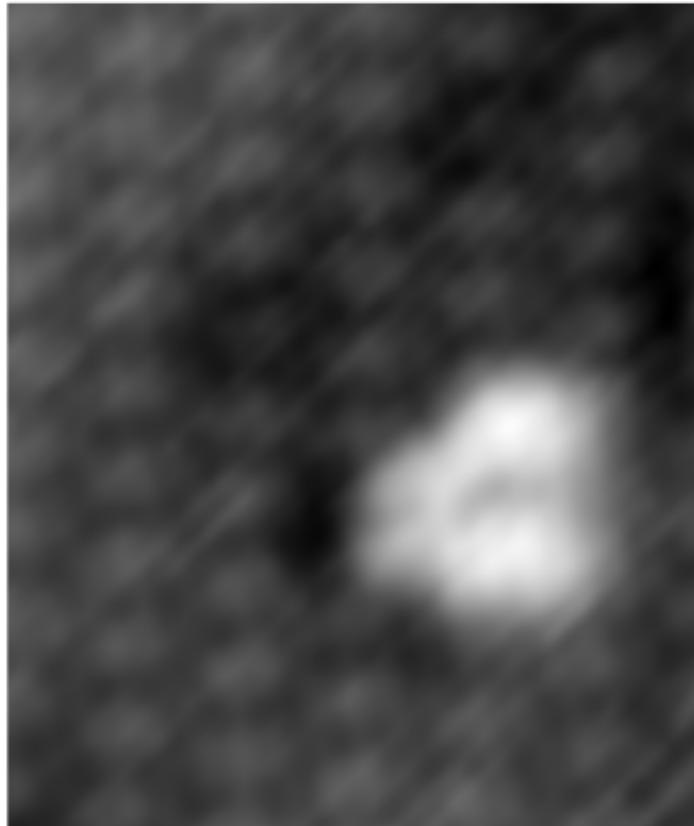


# Vanadium figures

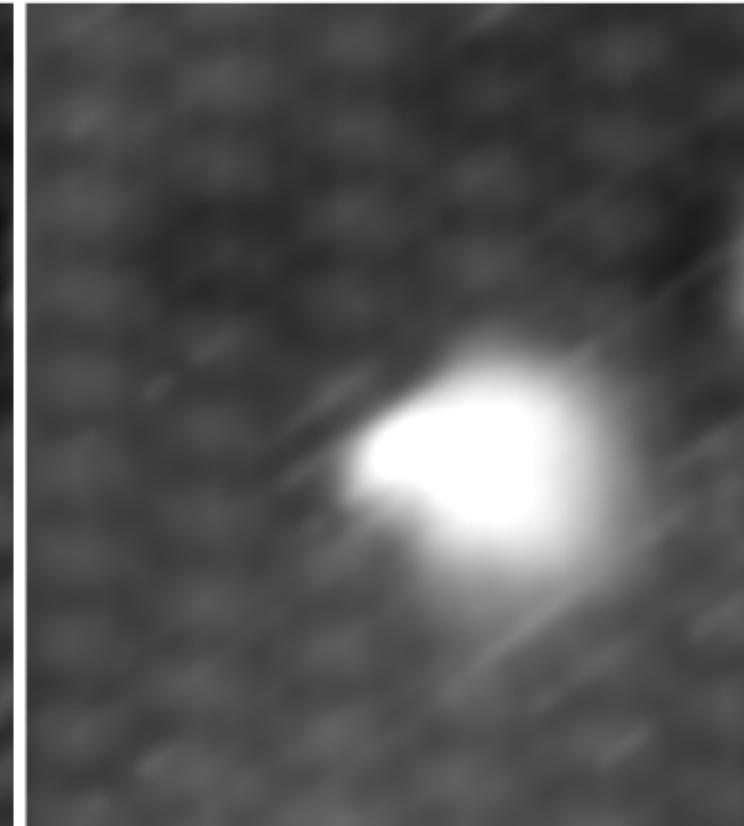
As-Deposited



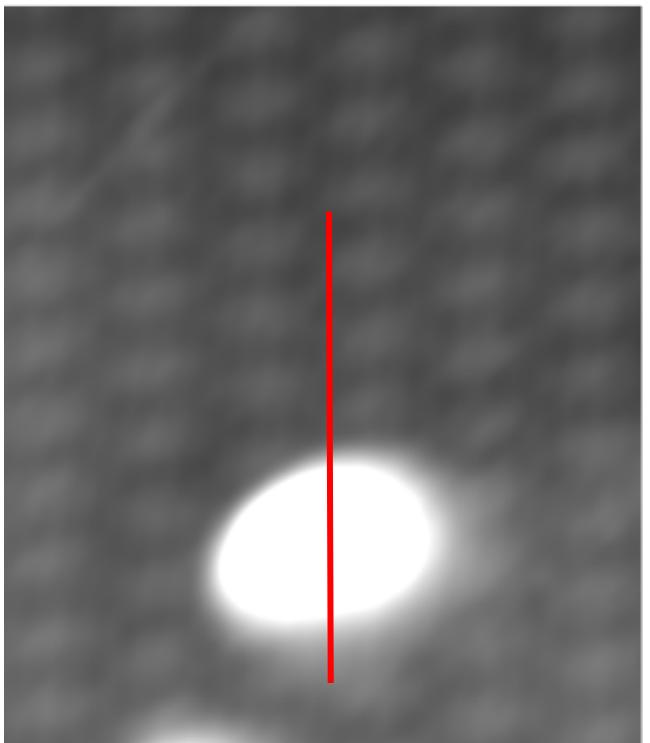
During Water exposure



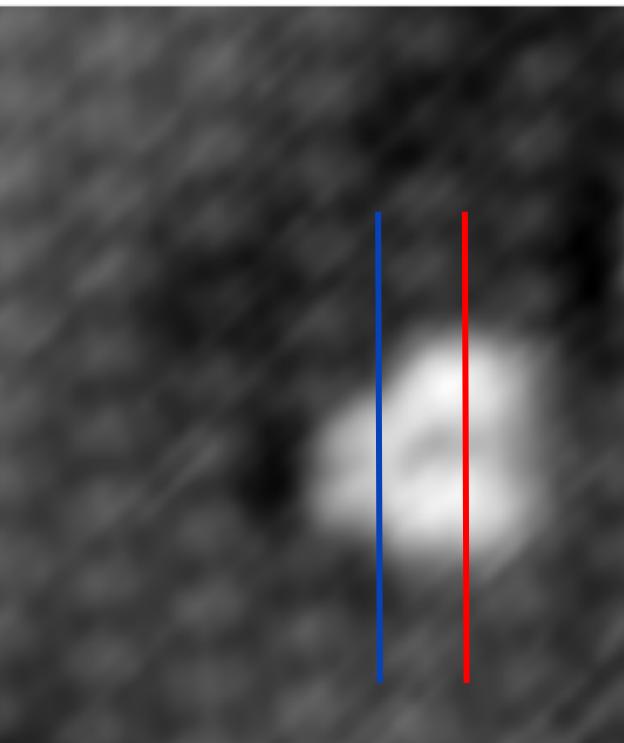
After Water Exposure



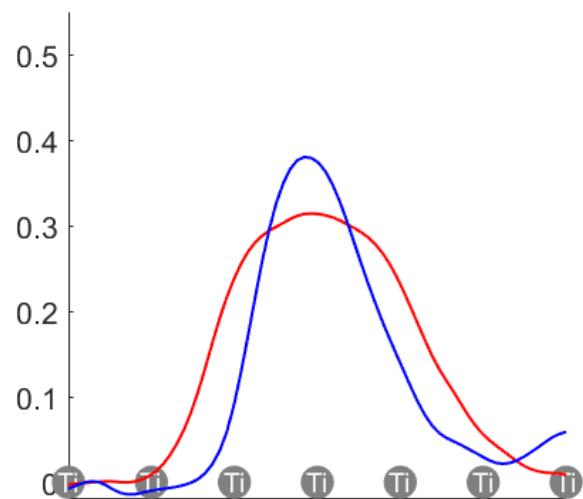
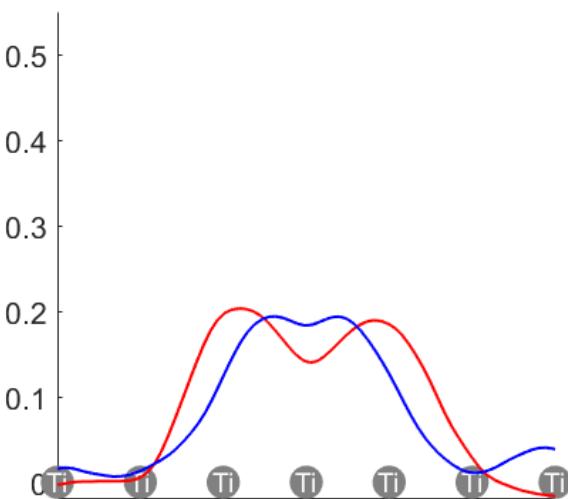
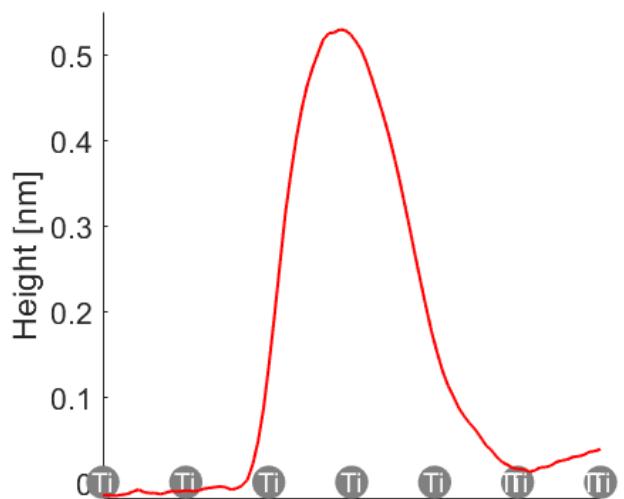
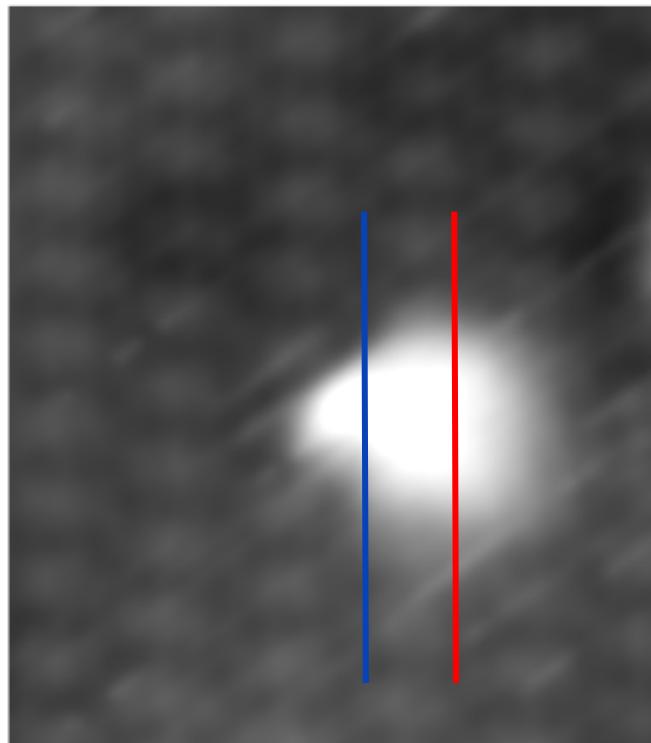
As-Deposited



During Water exposure



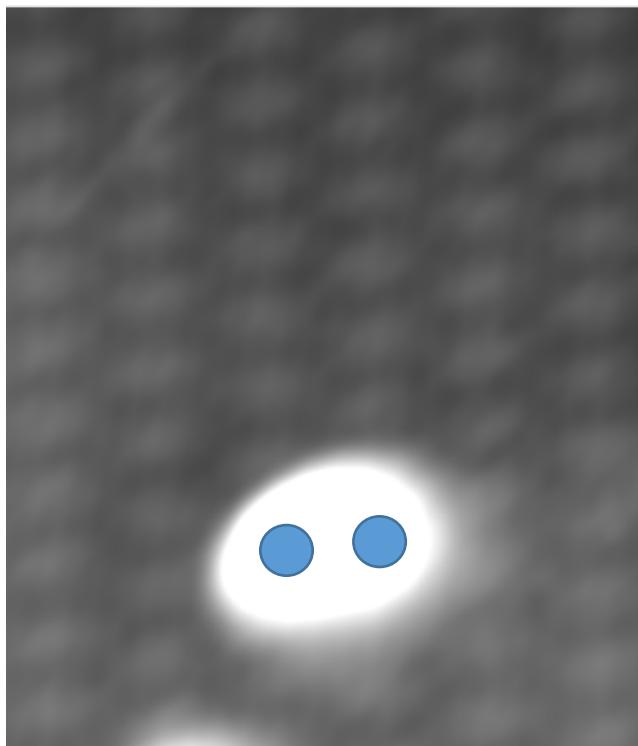
After Water Exposure



# model suggestions

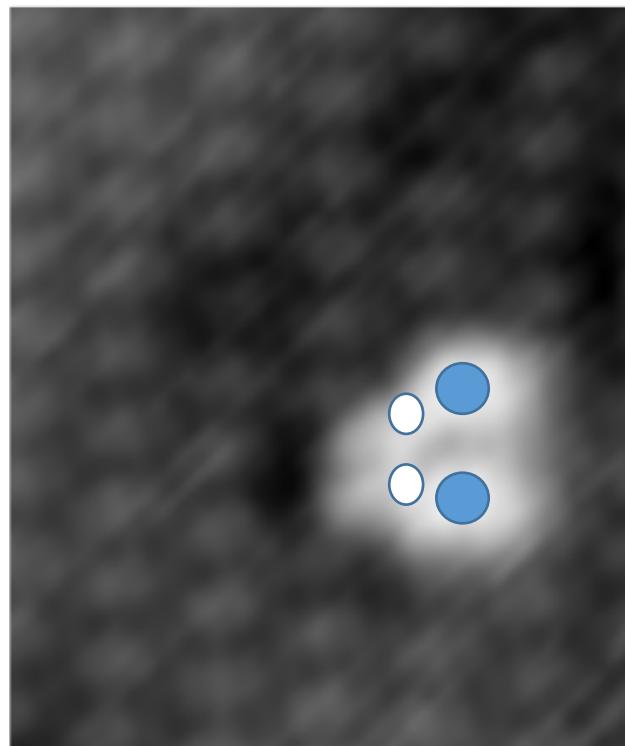
● = V

As-Deposited



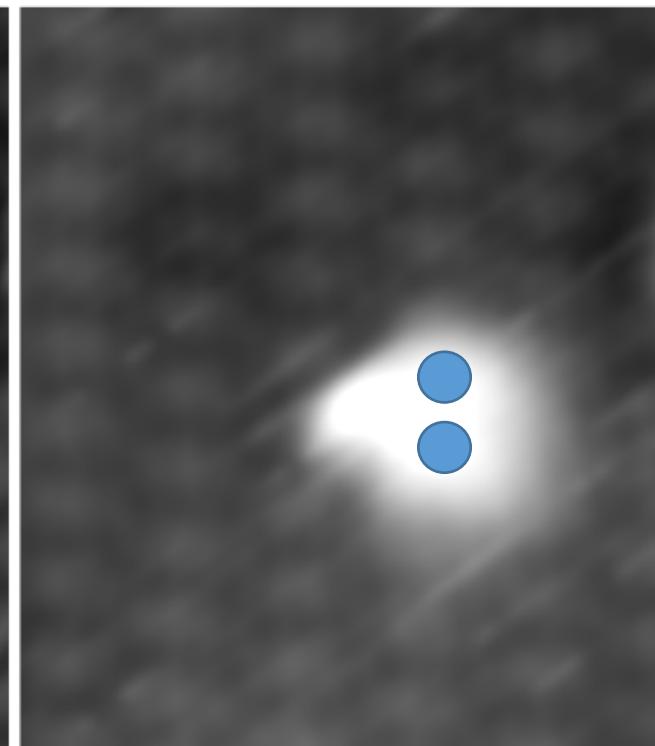
V2O5

During Water exposure



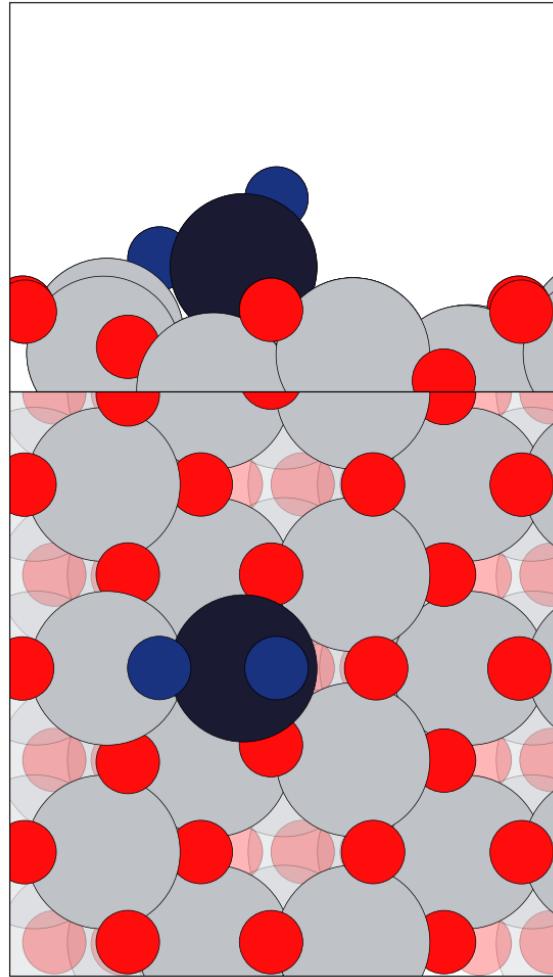
2 X VO<sub>3</sub>H

After Water Exposure



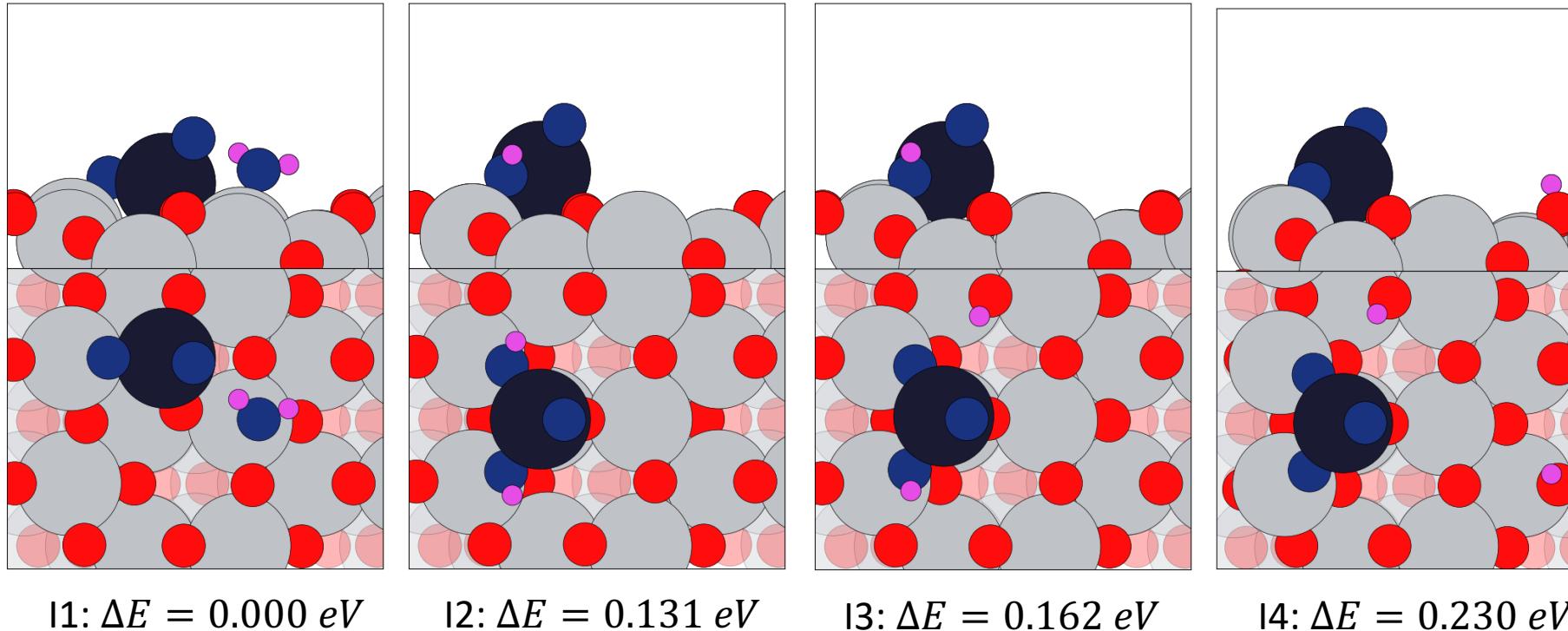
V2O5

# VO<sub>2</sub> Clusters with O<sub>v</sub> (1by2 Super cell)

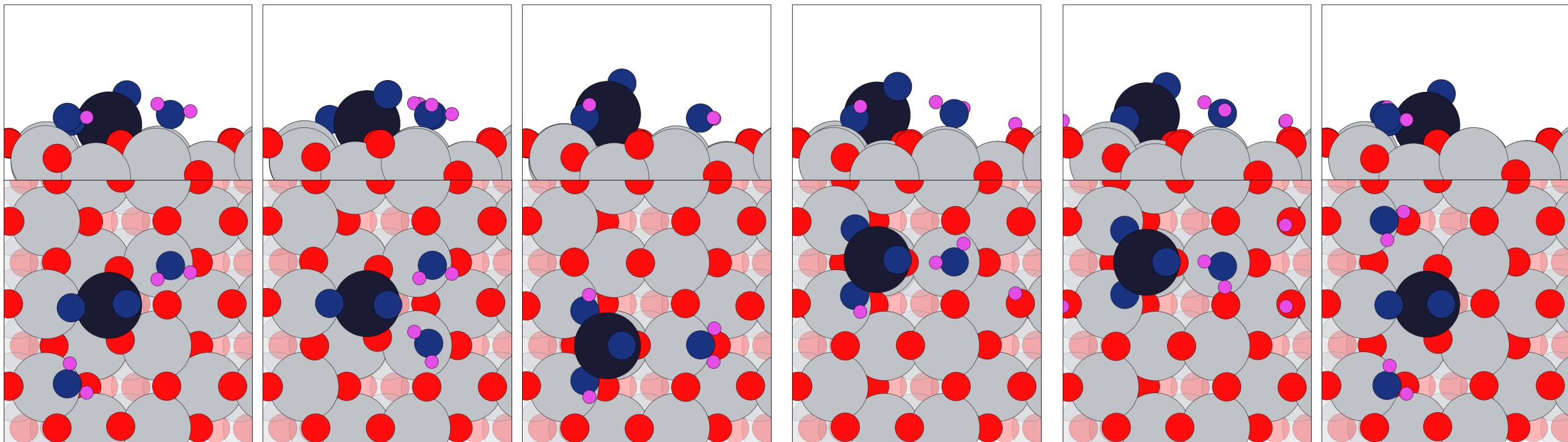


|1:  $\Delta E = 0.000 \text{ eV}$

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



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



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

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

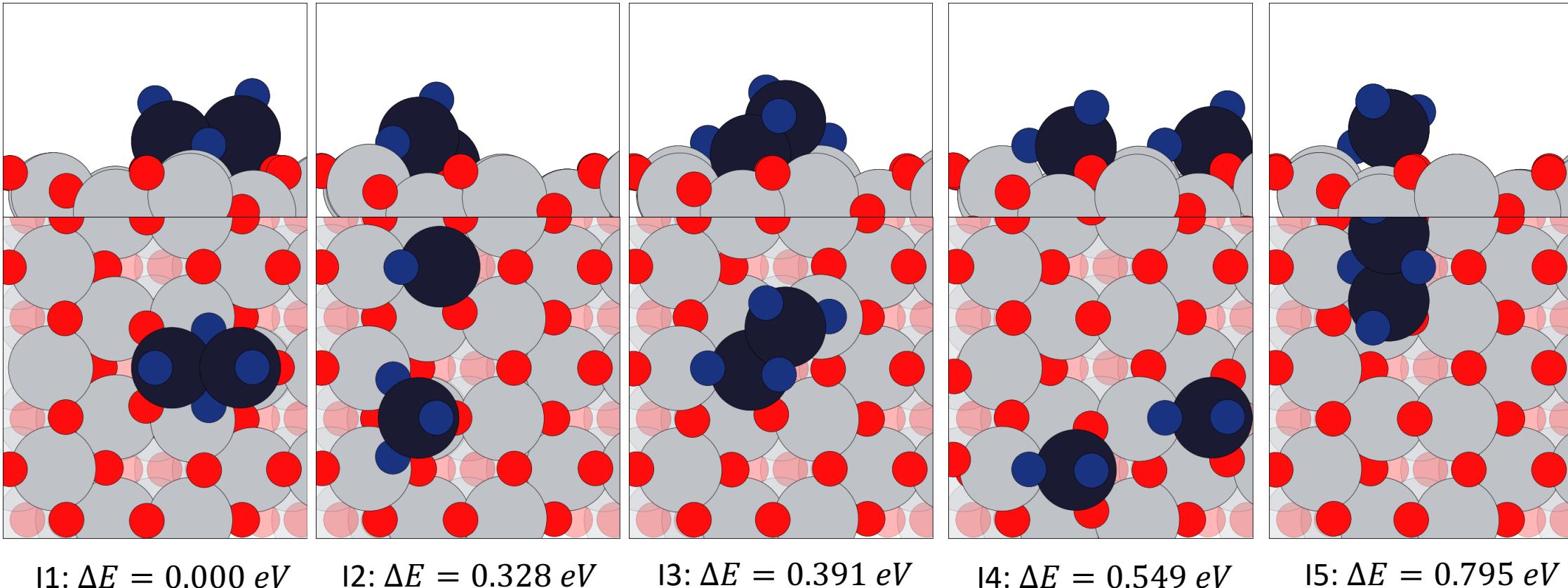
I3:  $\Delta E = 0.053 \text{ eV}$

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

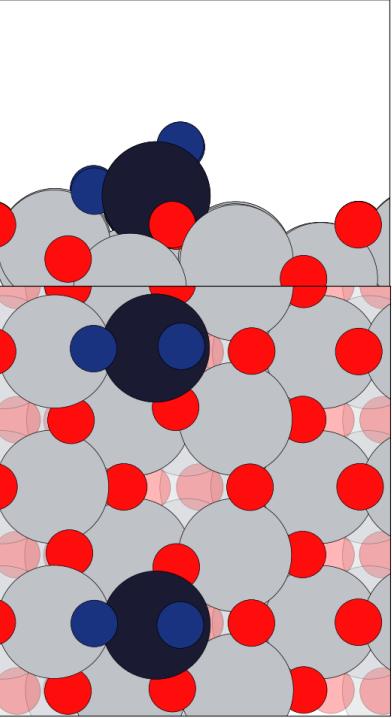
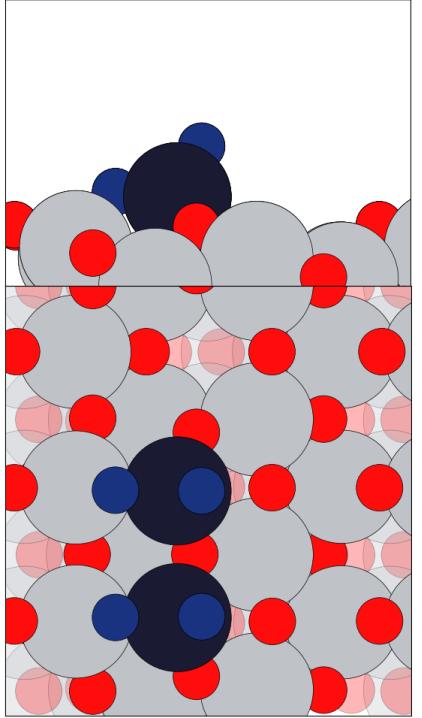
I5:  $\Delta E = 0.176 \text{ eV}$

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

# $V_2O_4$ Clusters with $O_v$ (1by3 Super cell)



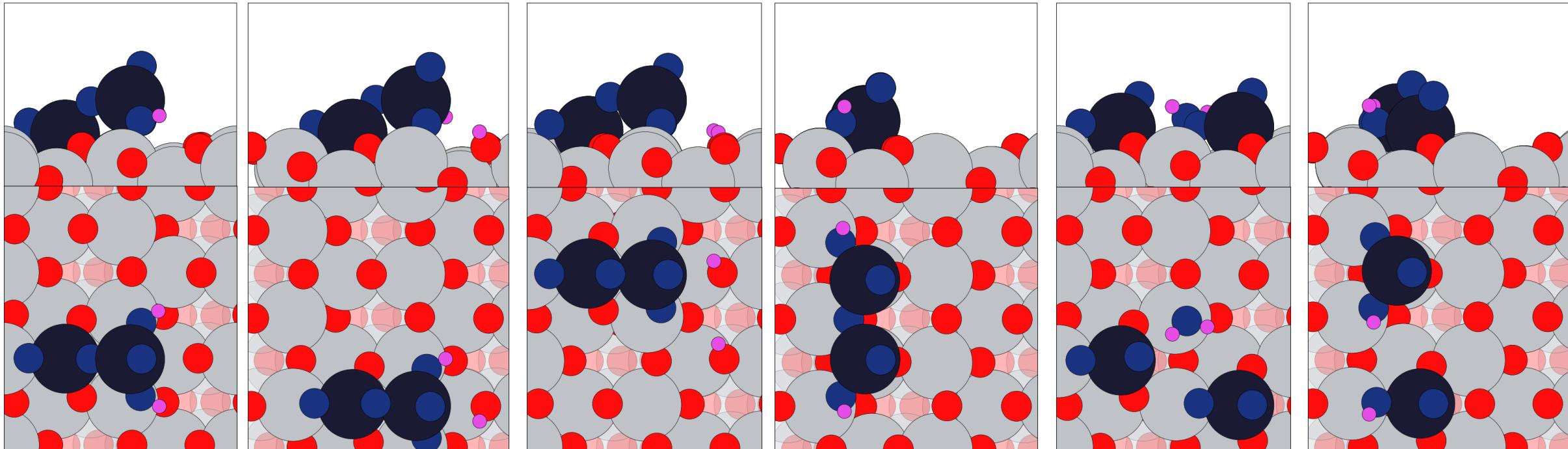
# $V_2O_4$ Clusters with $O_v$ (1by3 Super cell)



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 $\text{O}_v$ (1by3 Super cell)



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

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

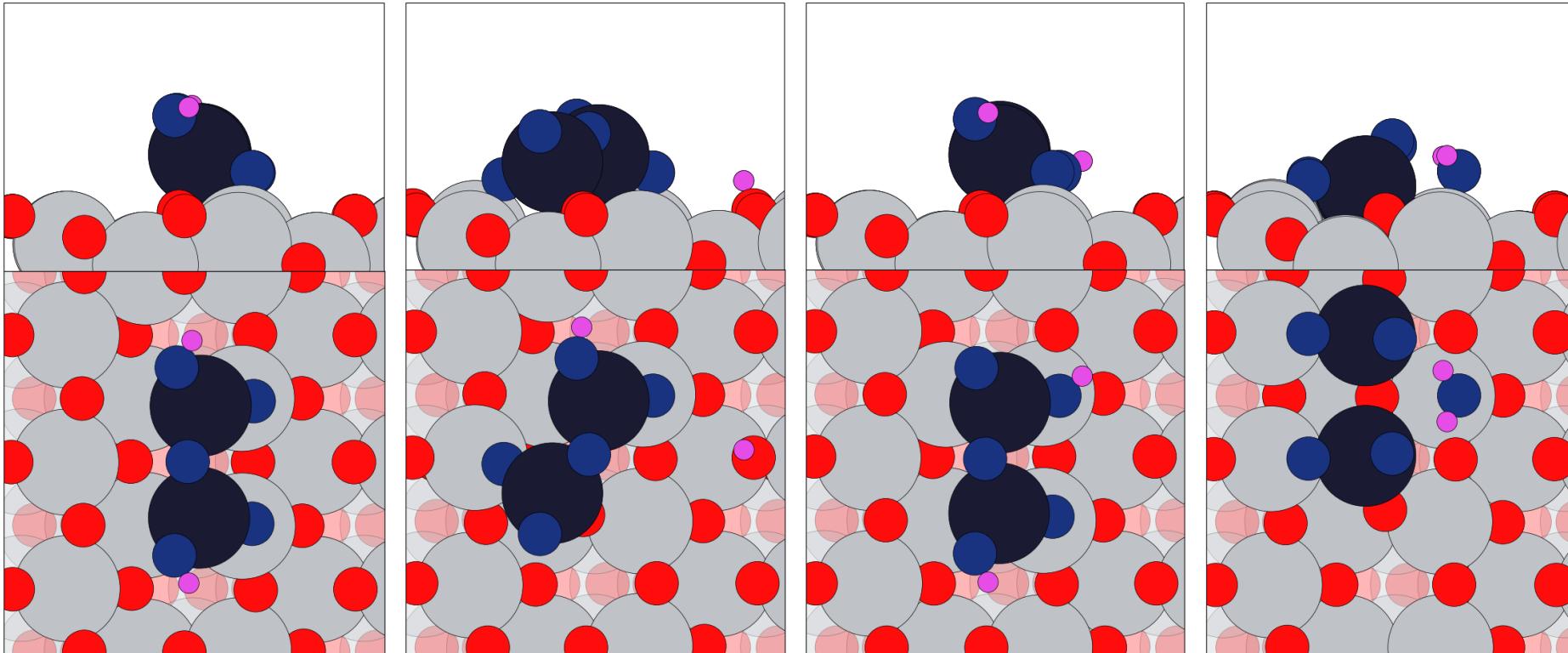
I3:  $\Delta E = 0.468 \text{ eV}$

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 $\text{O}_v$ (1by3 Super cell)



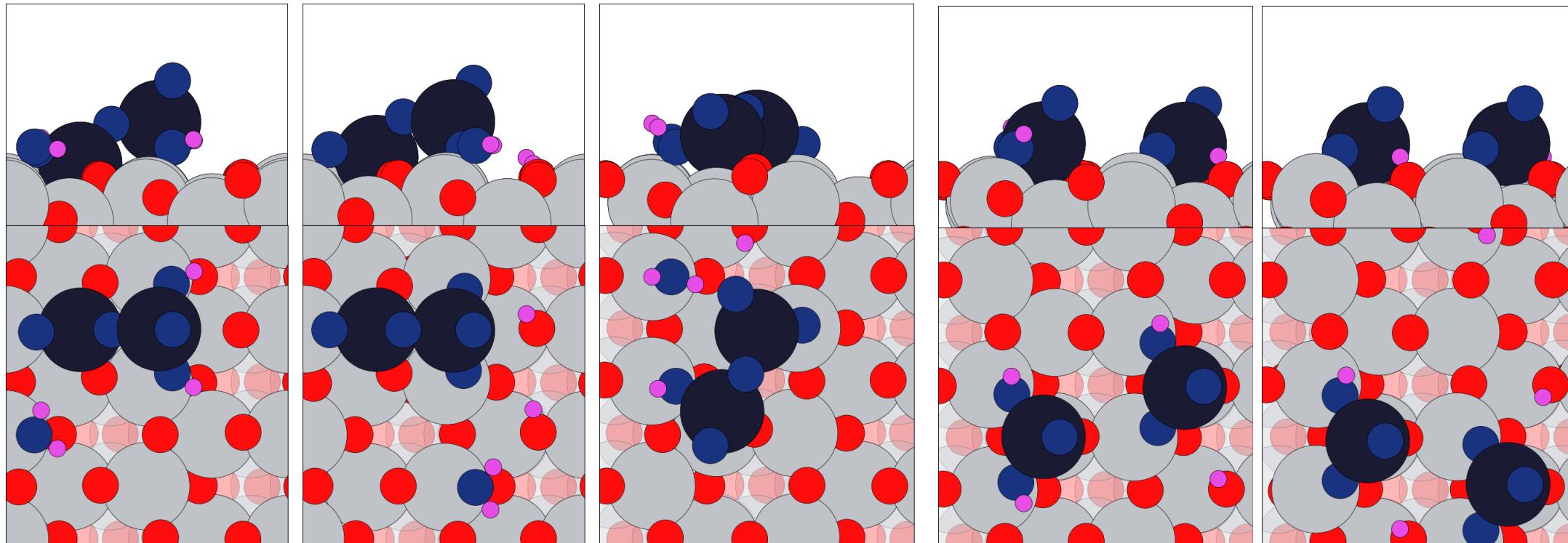
I7:  $\Delta E = 0.837 \text{ eV}$

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 $\text{O}_v$ (1by3 Super cell)



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

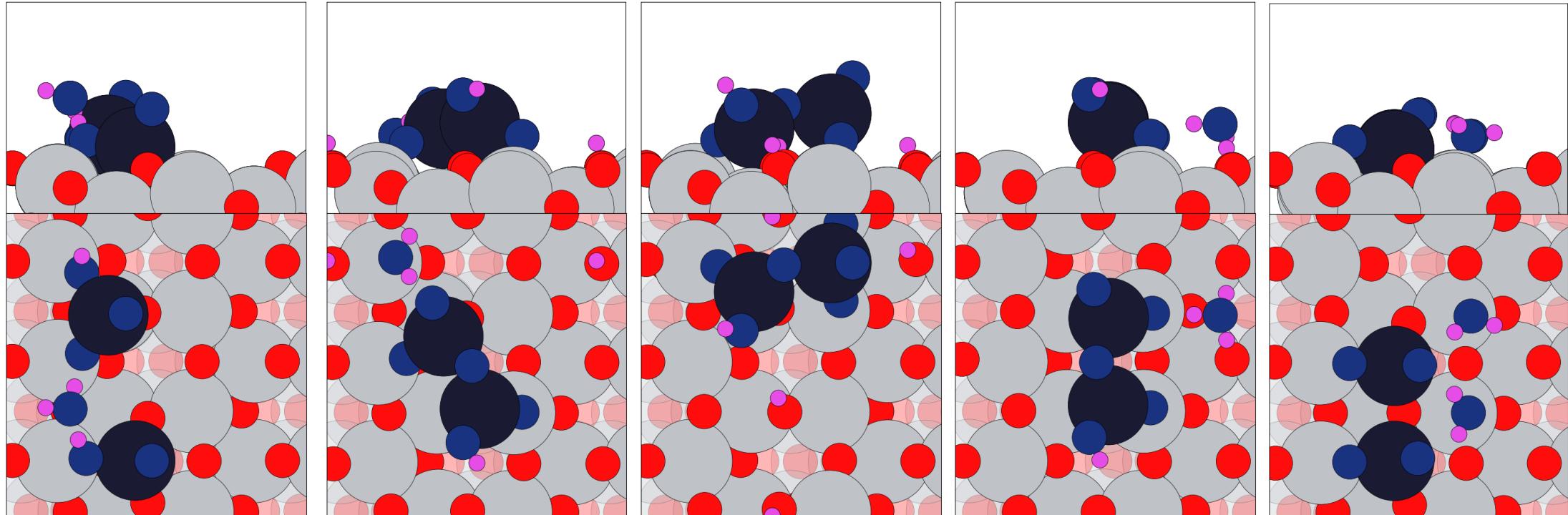
I2:  $\Delta E = 0.409 \text{ eV}$

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 $\text{O}_v$ (1by3 Super cell)



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

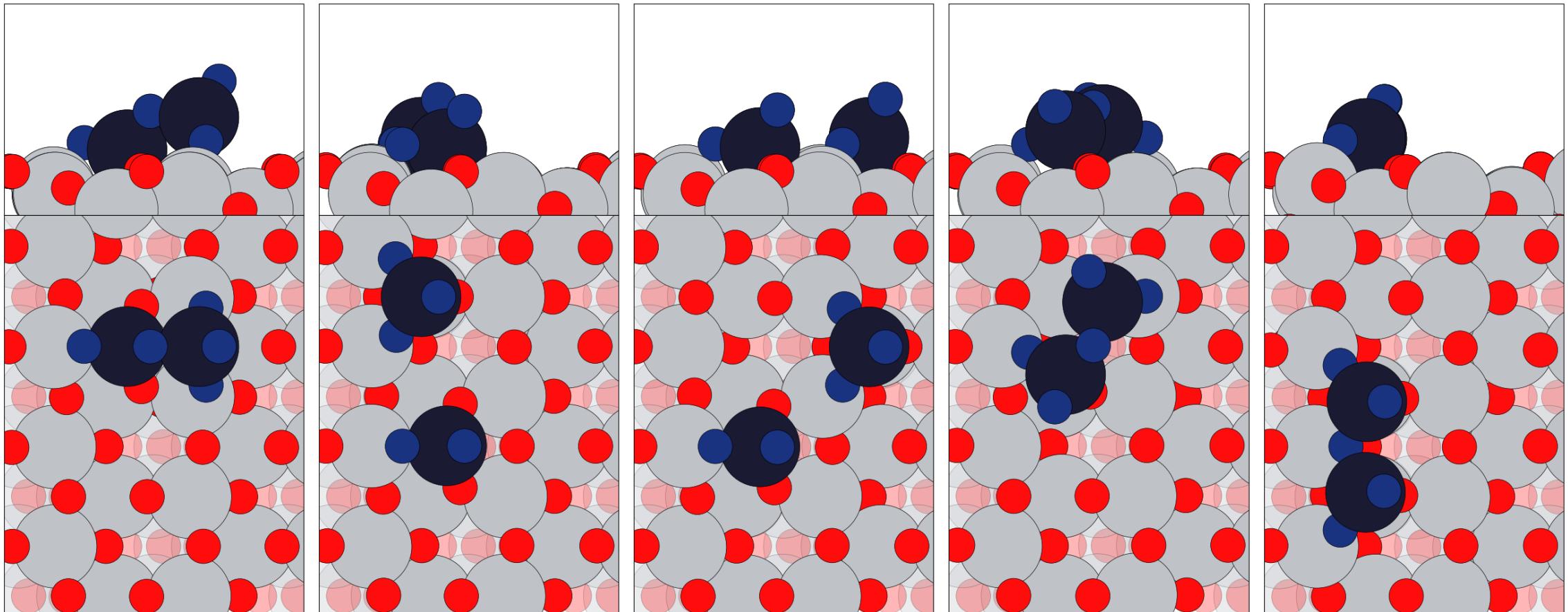
I7:  $\Delta E = 0.837 \text{ eV}$

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

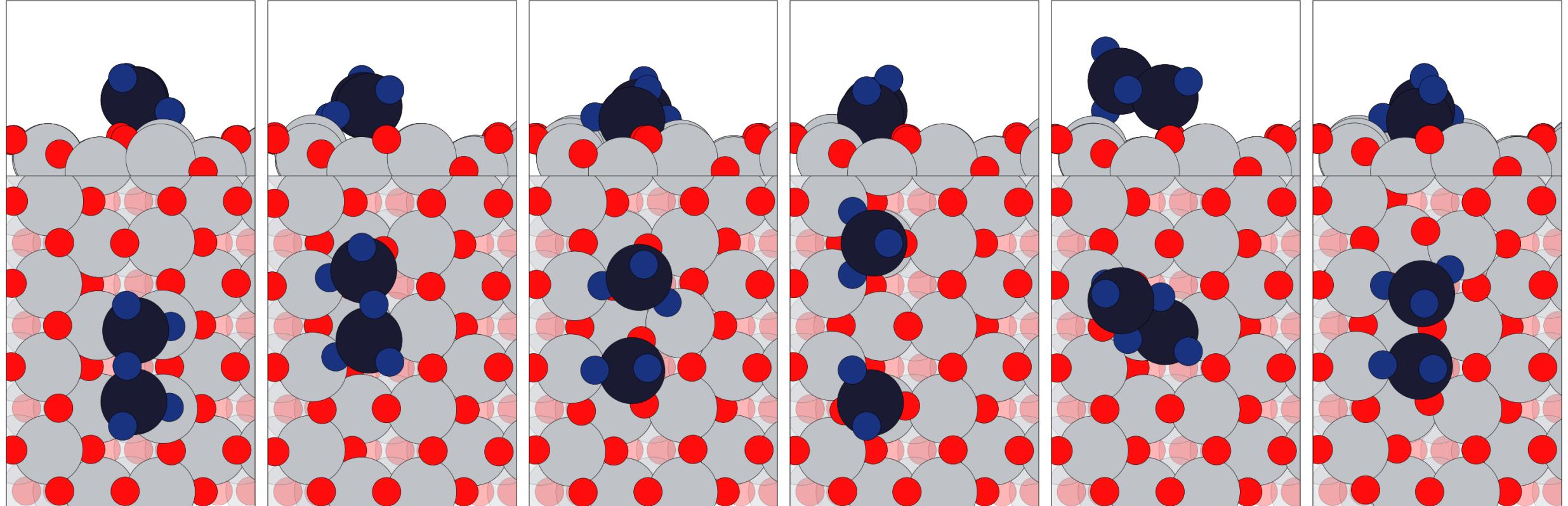
I2:  $\Delta E = 0.127 \text{ eV}$

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

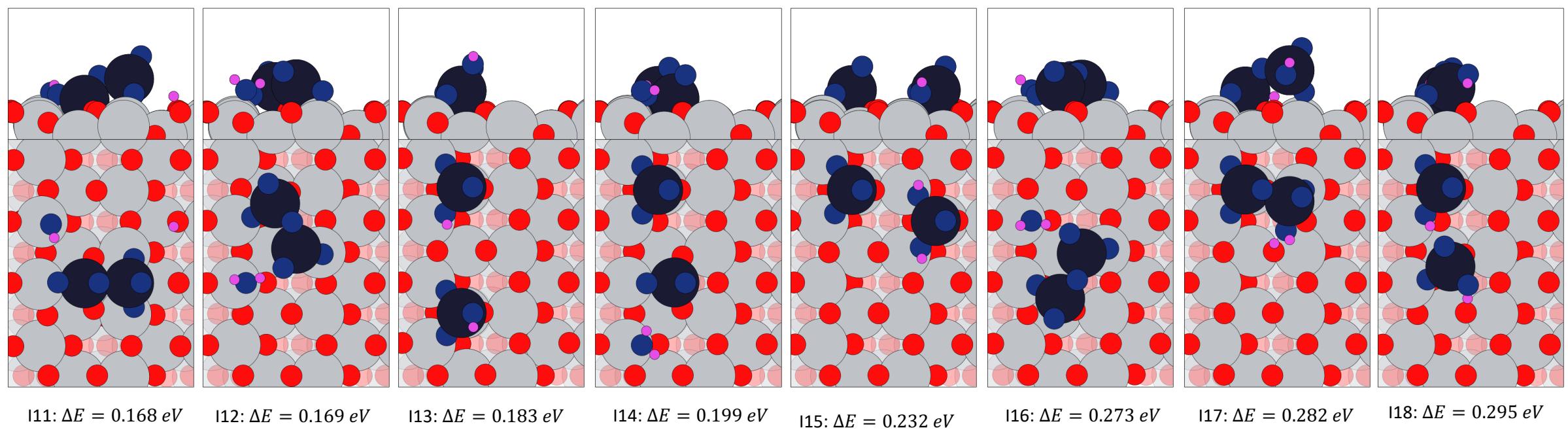
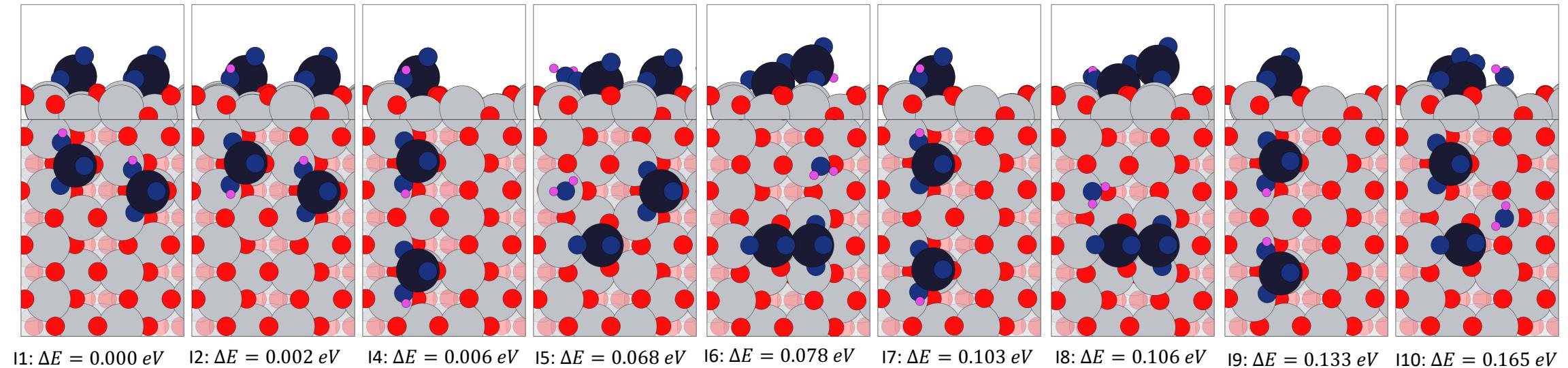
I9:  $\Delta E = 1.164 \text{ eV}$

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

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

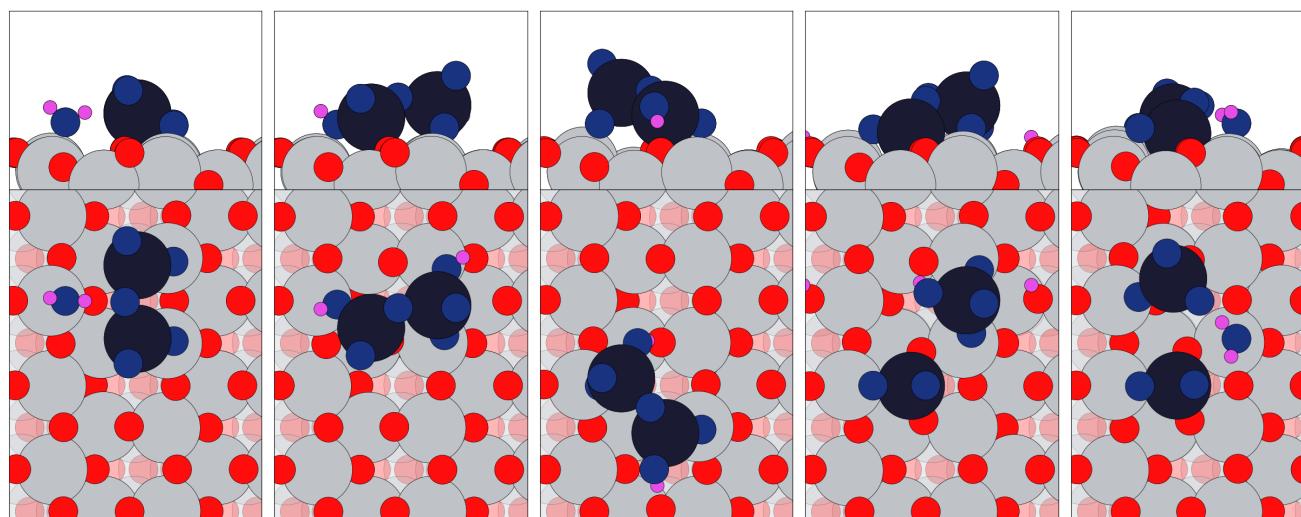
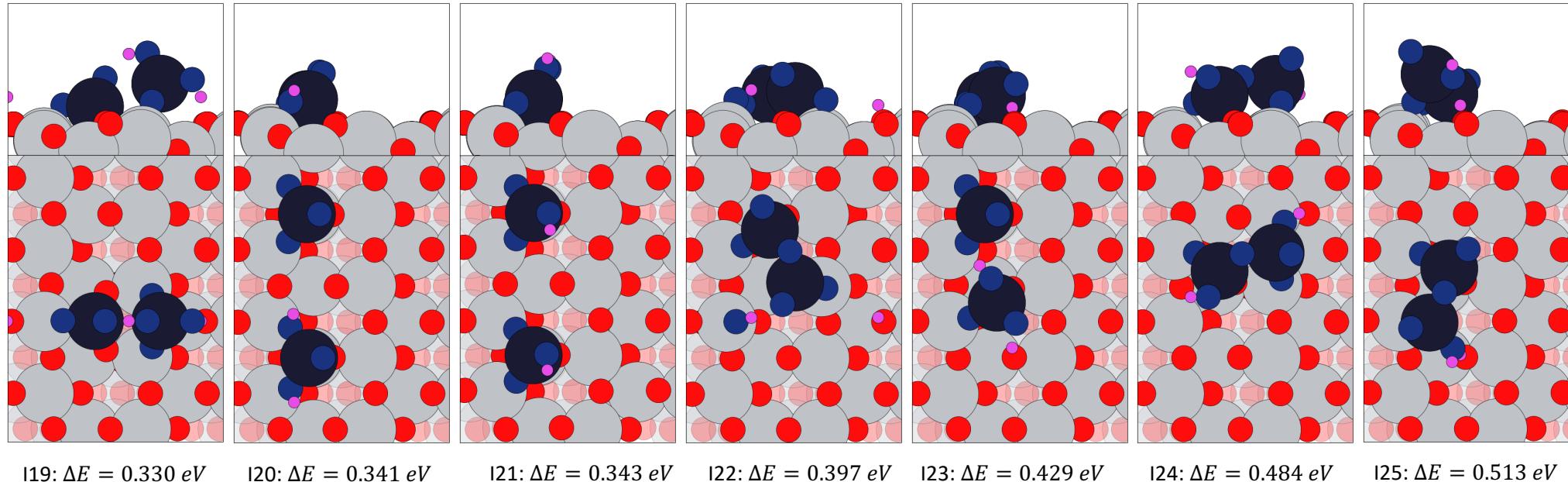
## $V_2O_5$ Clusters with $O_v$ (1by4 cell)

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



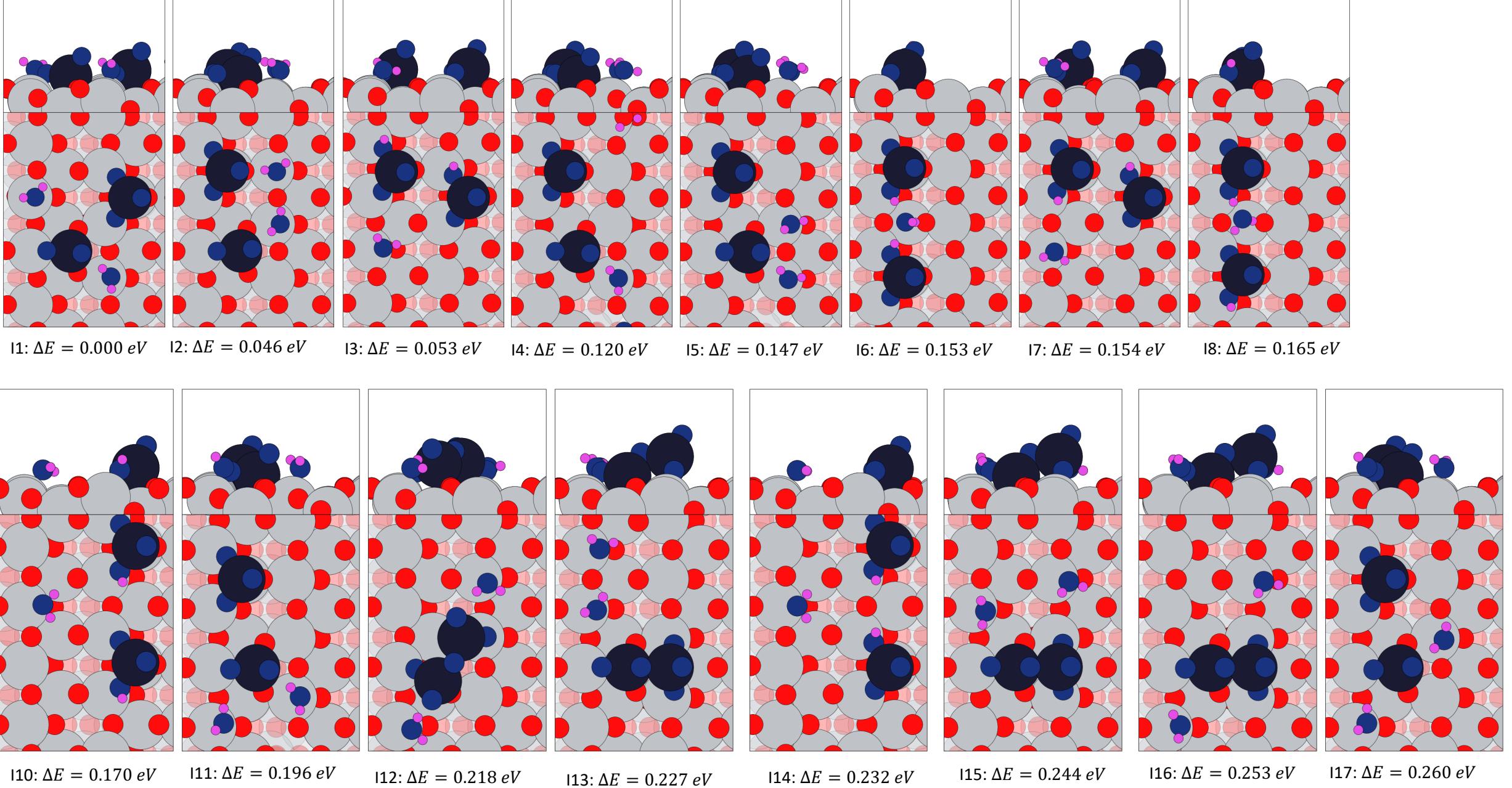
## $V_2O_5$ Clusters with $O_v$ (1by4 cell)

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



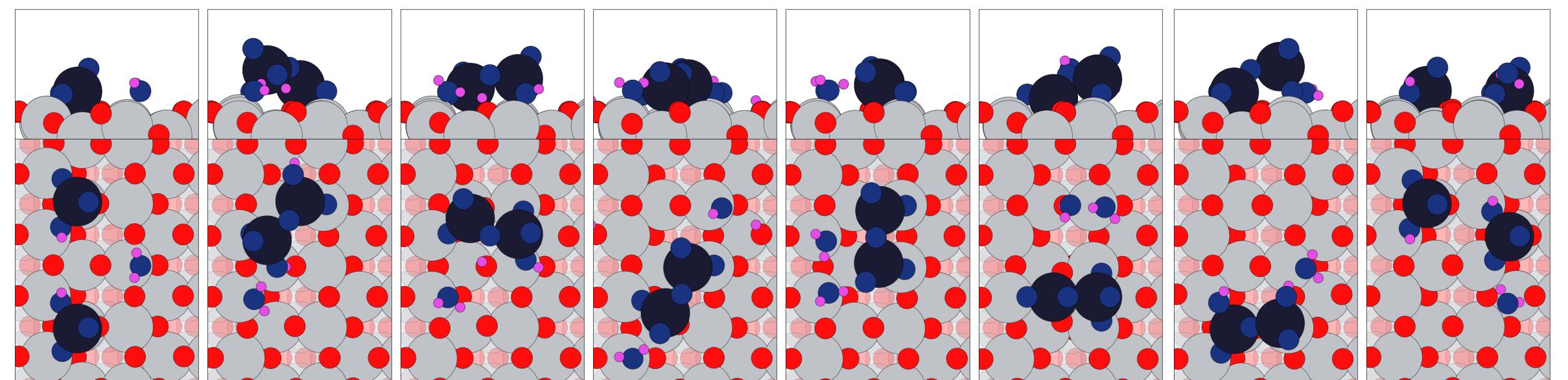
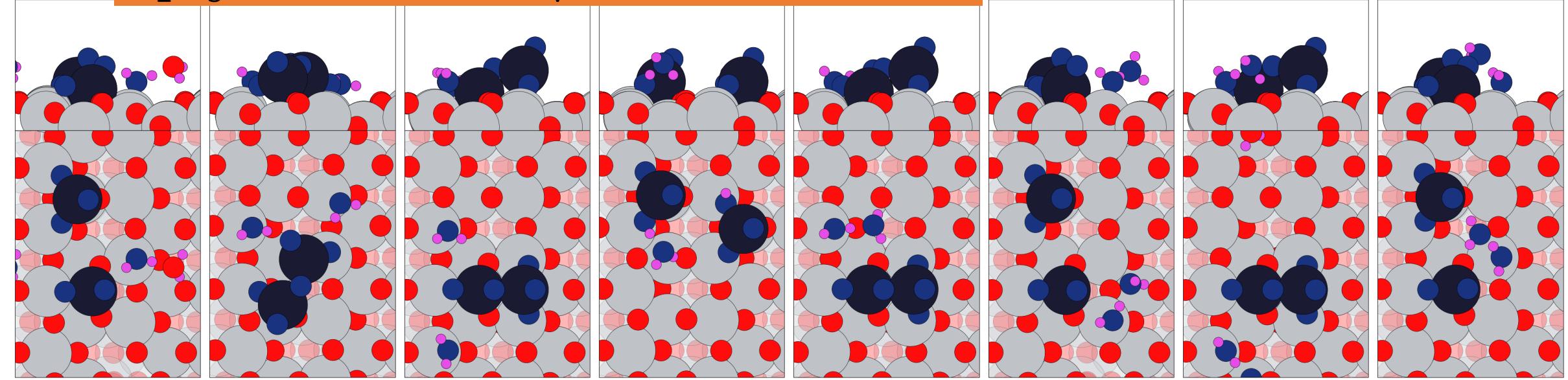
# $V_2O_5$ Clusters with $O_v$ (1by4 Super cell)

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



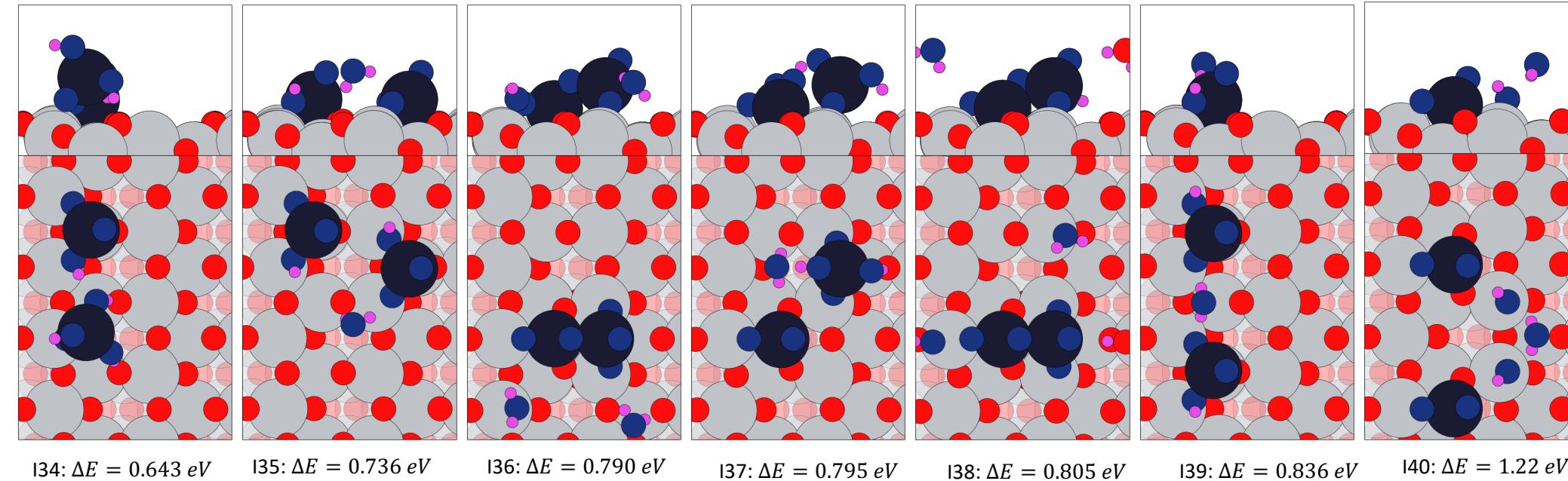
# $V_2O_5$ Clusters with $O_v$ (1by4 Super cell)

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



# $V_2O_5$ Clusters with $O_v$ (1by4 Super cell)

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



# GPAW and CP2K

## GPAW

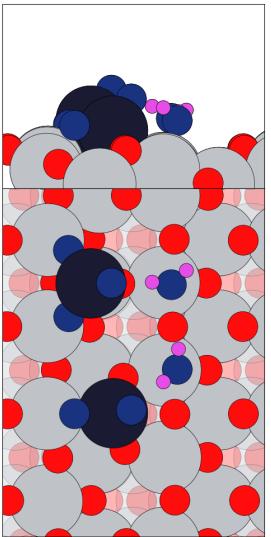
Mode = PW

E\_cut = 500 eV for plane wave

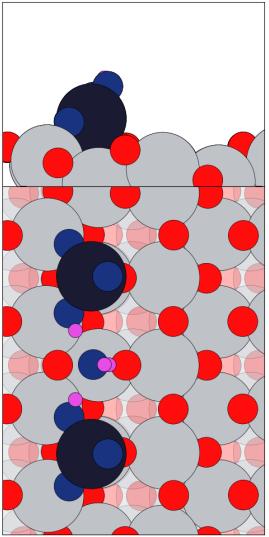
XC = PBE

U\_corr (Hubbard term) = 4.0 eV

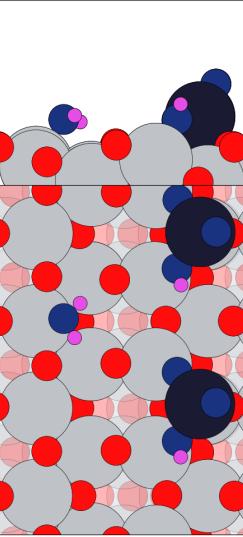
F\_cut = 0.025 eV/Ang



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



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



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

## CP2K

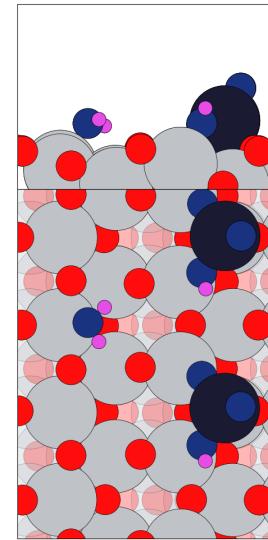
Mode = GPW (gaussian and plane wave method)

E\_cut = 400 Ry for plane wave

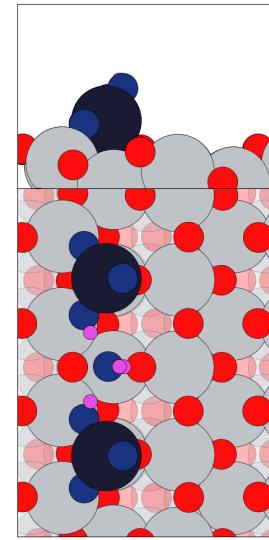
XC = PBE

Dispersion correction = DFTD3 (PBE functional)

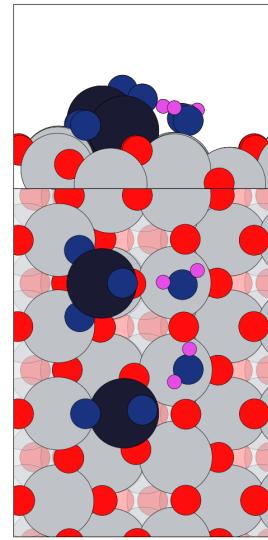
F\_cut = 0.023 eV/Ang



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

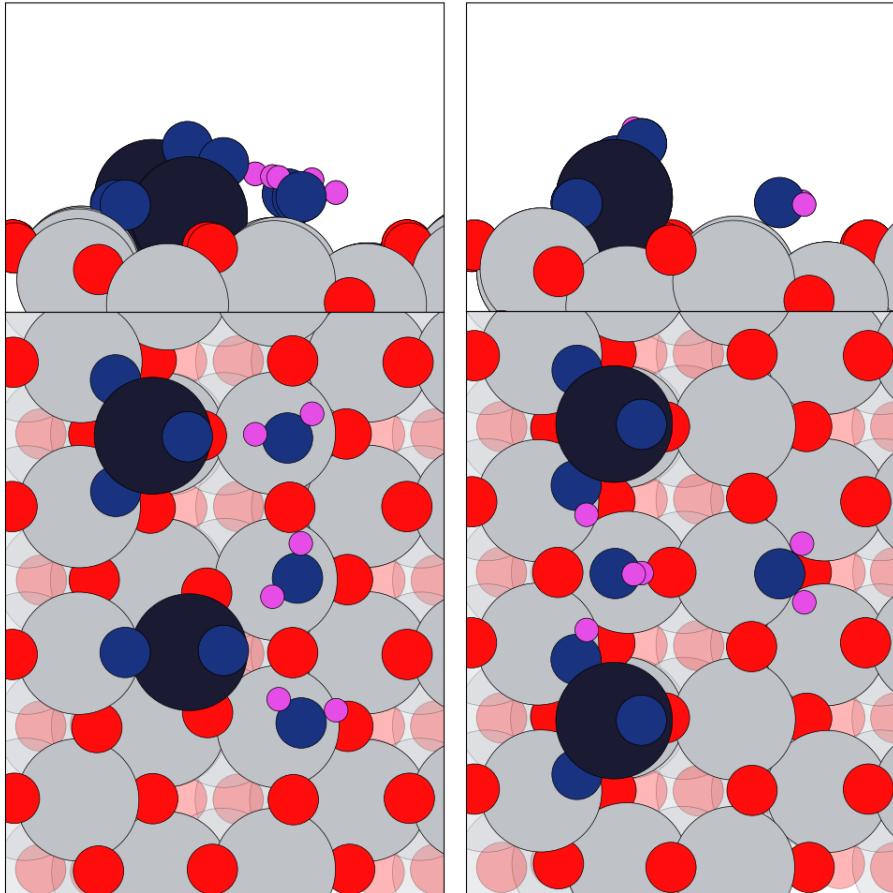
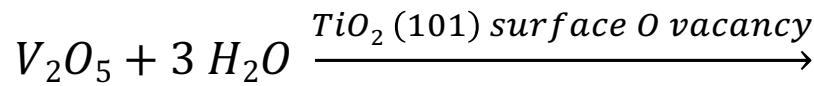


I2:  $\Delta E = 0.13 \text{ eV}$



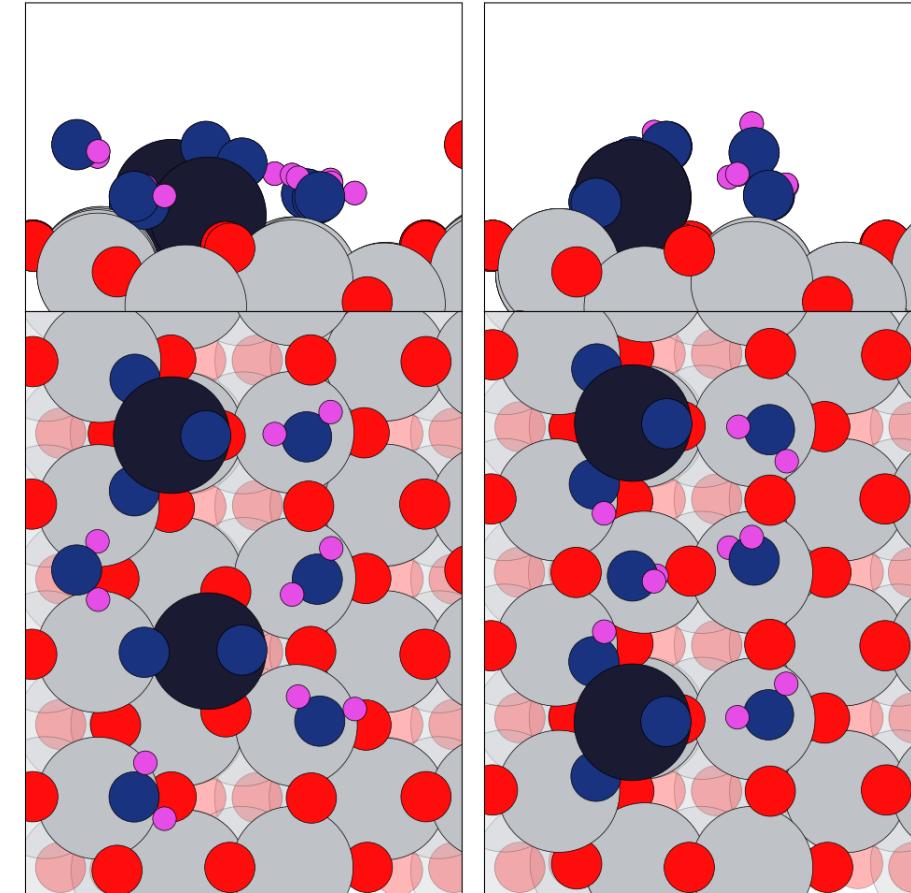
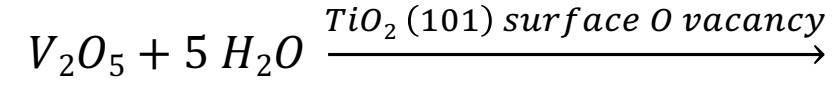
I3:  $\Delta E = 0.71 \text{ eV}$

# $V_2O_5$ Clusters with $O_v$ (1by4 Super cell)



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

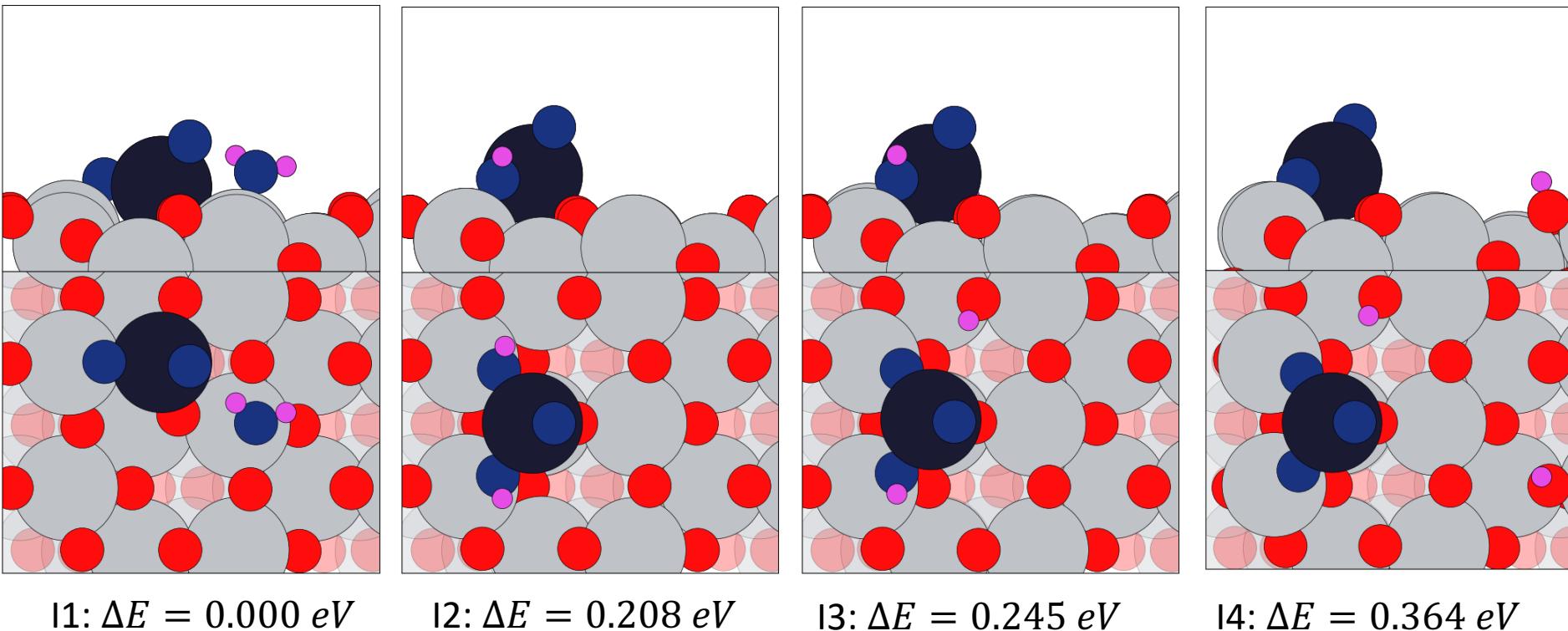
|2:  $\Delta E = 0.272 \text{ eV}$



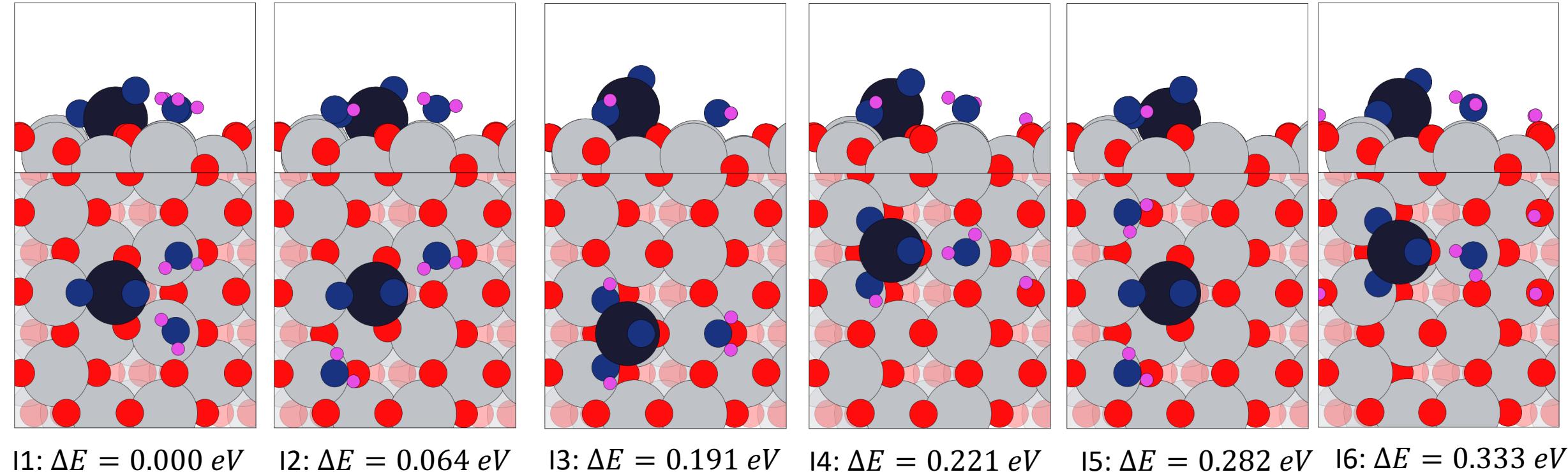
|1:  $\Delta E = 0.000 \text{ eV}$

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

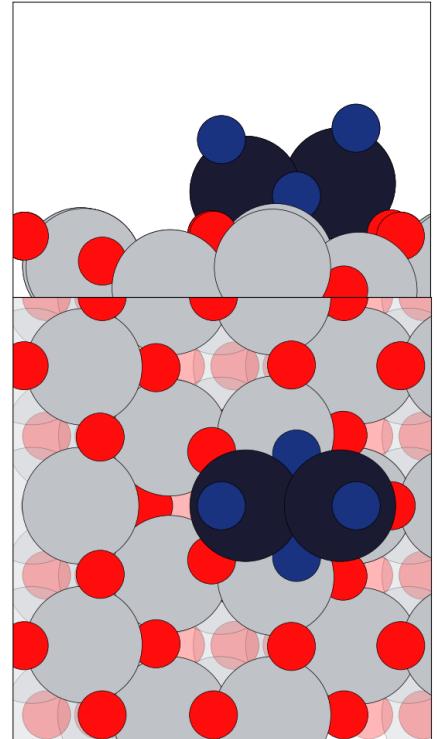
# $\text{VO}_2 + \text{H}_2\text{O}$ Clusters (1by2 Super cell)



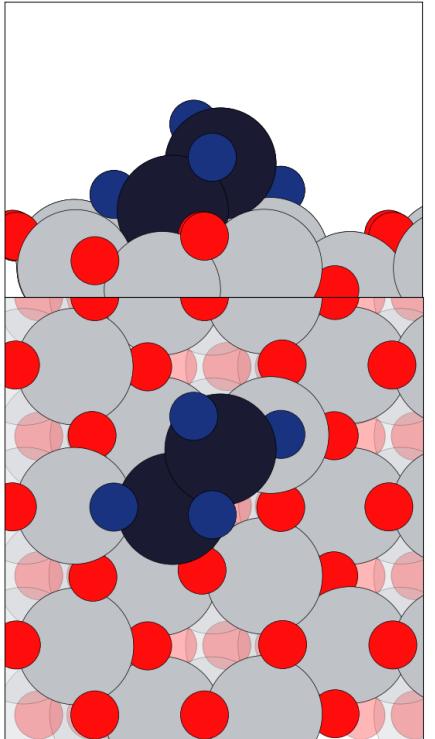
# $\text{VO}_2 + 2\text{H}_2\text{O}$ Clusters (1by3 Super cell)



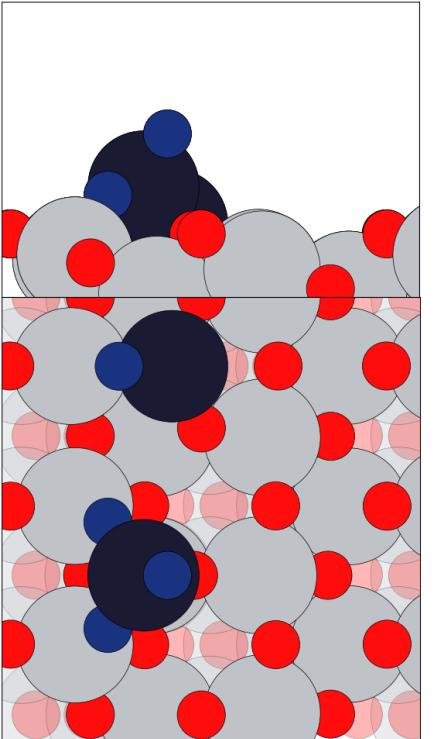
# $\text{V}_2\text{O}_4$ Clusters (1by3 Super cell)



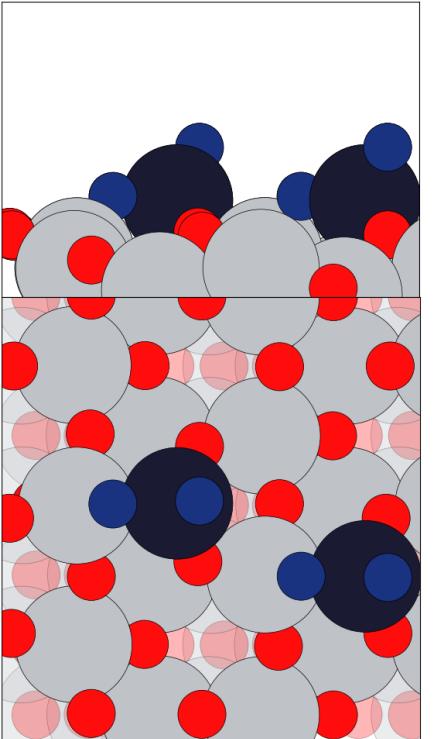
I1:  $\Delta E = 0.000 \text{ eV}$



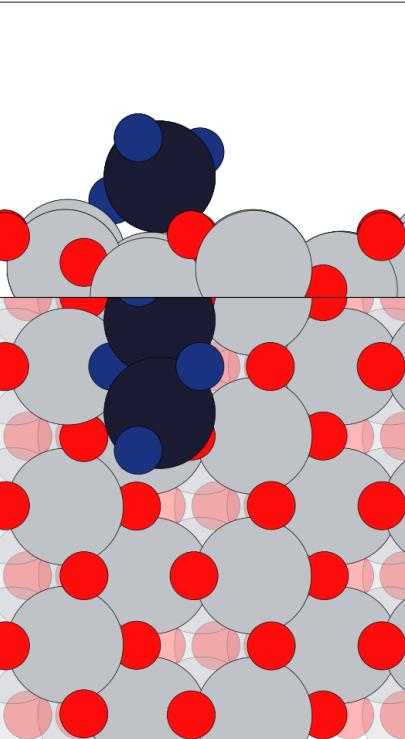
I2:  $\Delta E = 0.207 \text{ eV}$



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

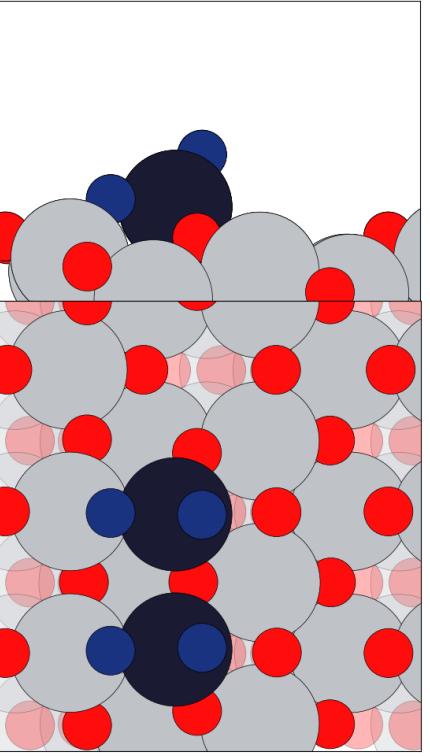
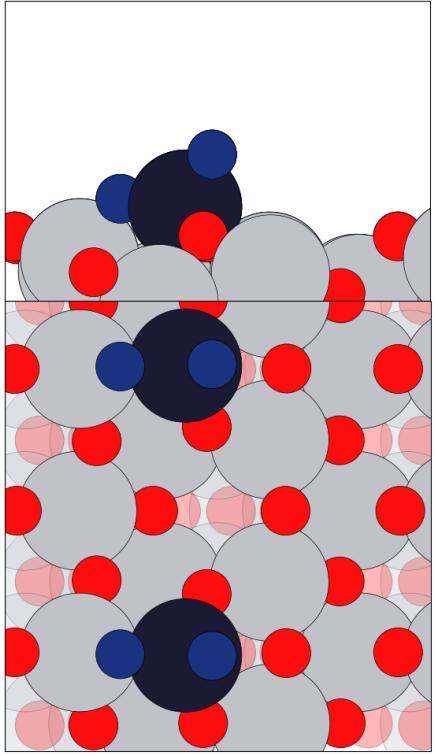


I4:  $\Delta E = 0.466 \text{ eV}$



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

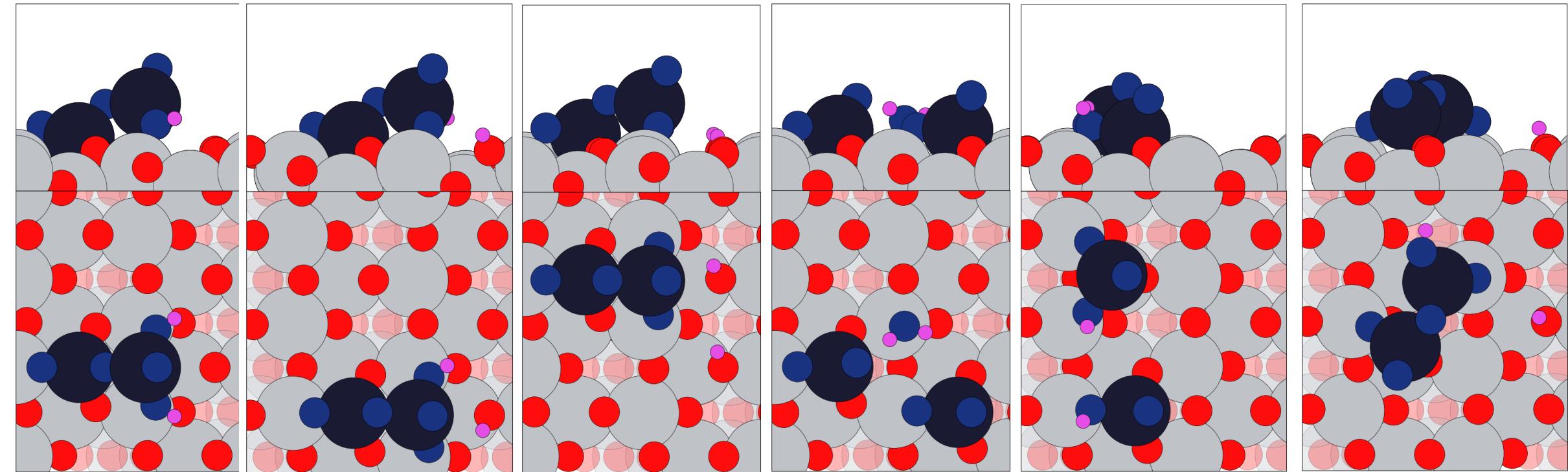
# $\text{V}_2\text{O}_4$ Clusters (1by3 Super cell)



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

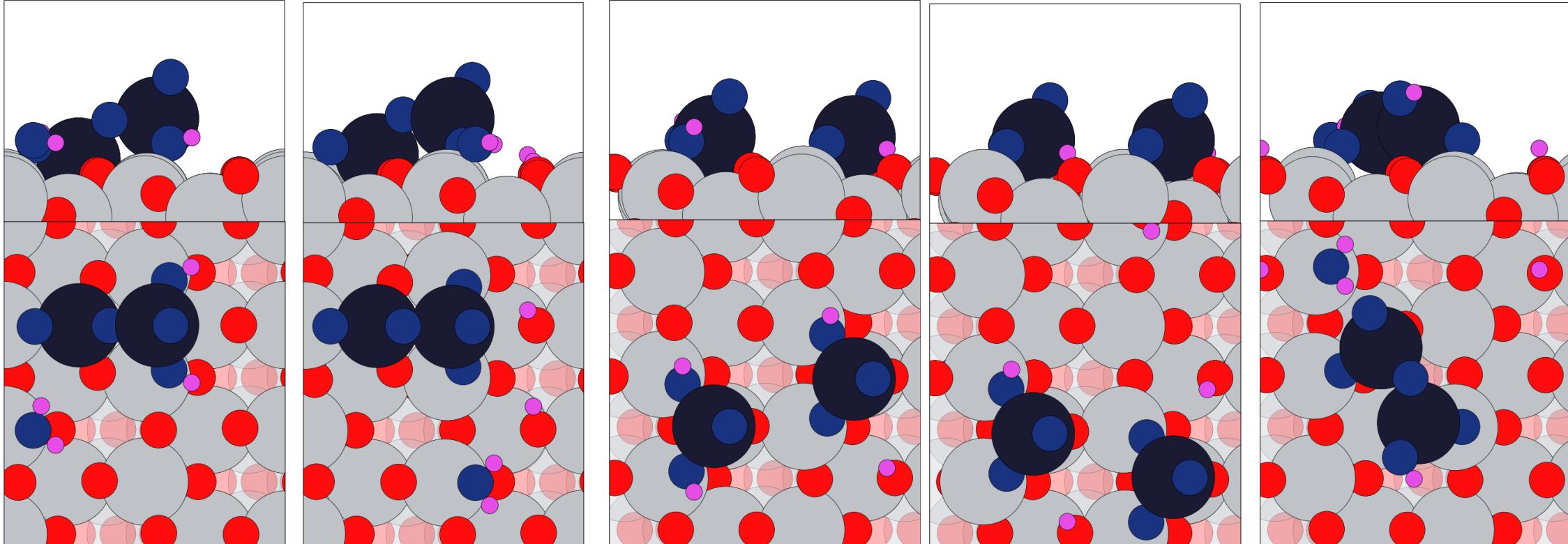
I7:  $\Delta E = 1.101 \text{ eV}$

# $\text{V}_2\text{O}_4 + \text{H}_2\text{O}$ 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:  $\Delta E = 0.000 \text{ eV}$

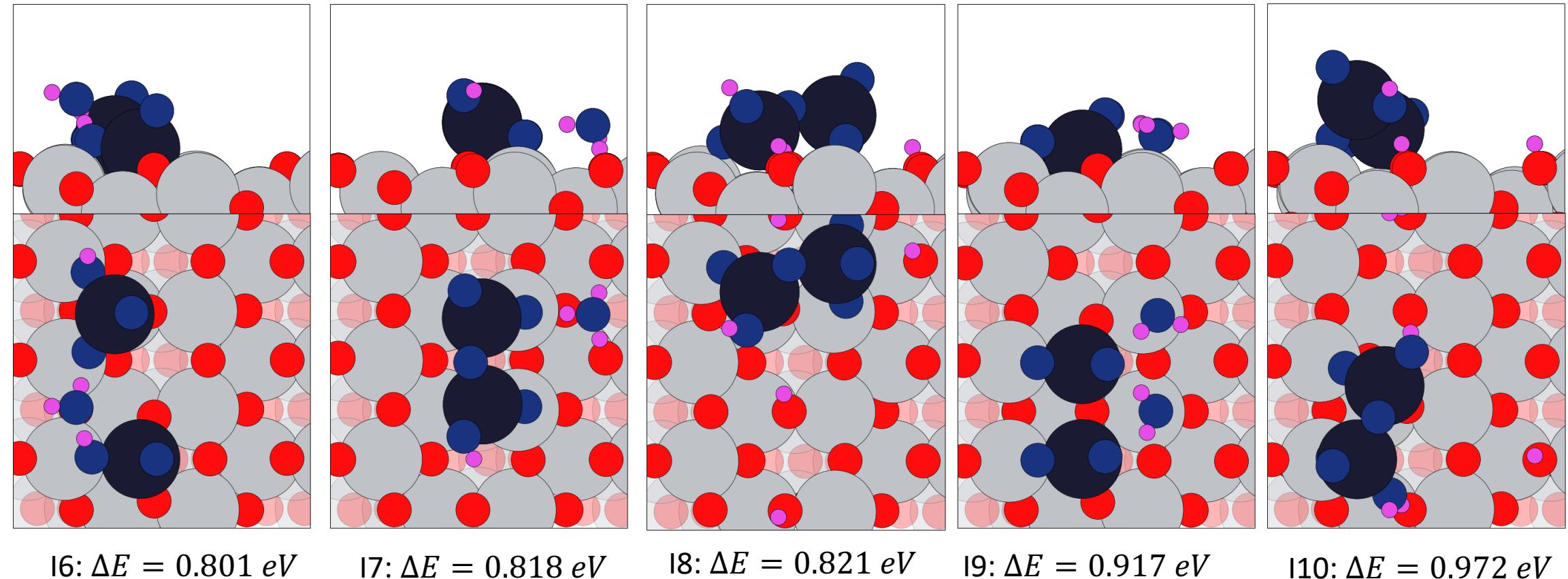
I2:  $\Delta E = 0.436 \text{ eV}$

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

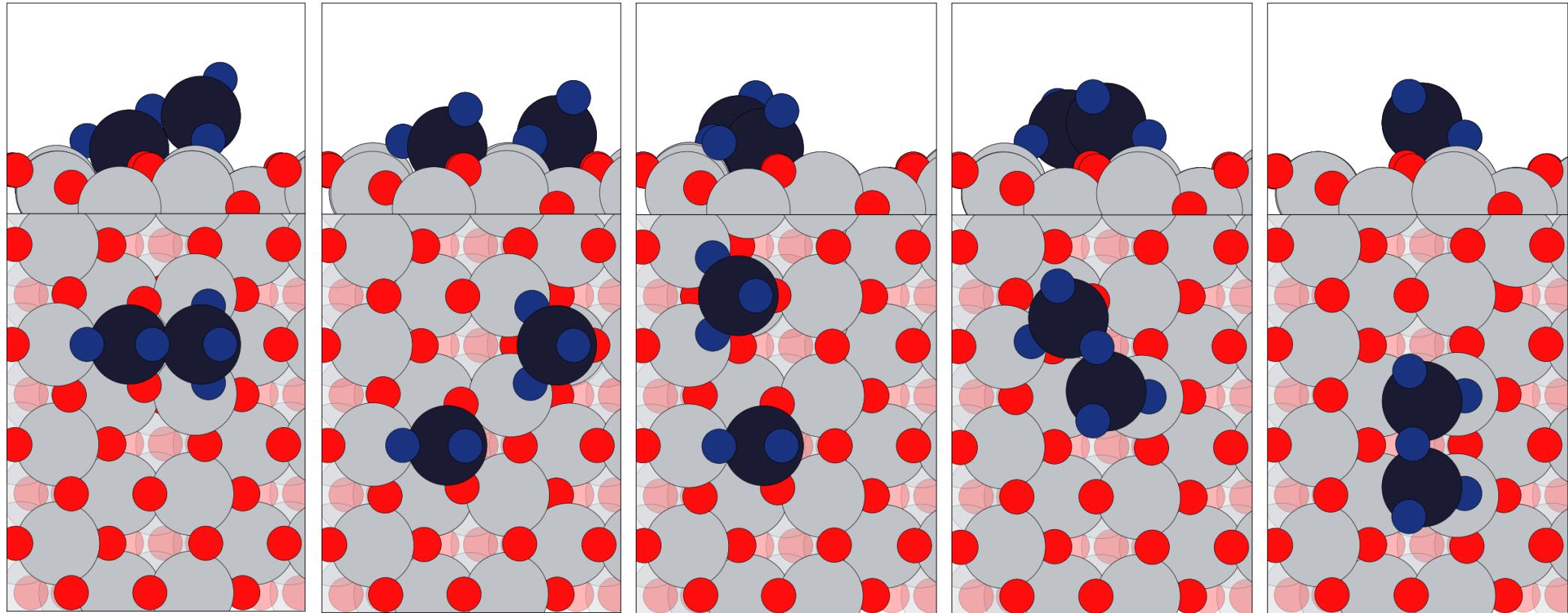
I4:  $\Delta E = 0.642 \text{ eV}$

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

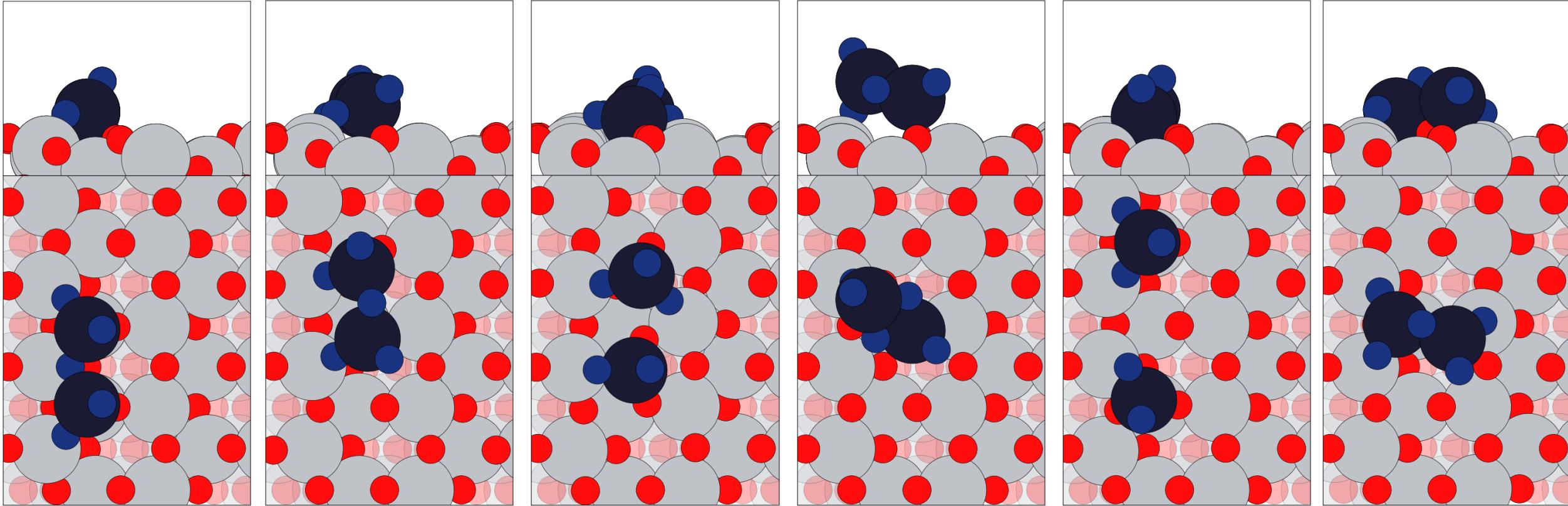
# $\text{V}_2\text{O}_4 + 2\text{H}_2\text{O}$ Clusters (1by3 Super cell)



# $\text{V}_2\text{O}_5$ Clusters (1by4 Super cell)



# $V_2O_5$ Clusters (1by4 Super cell)



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

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

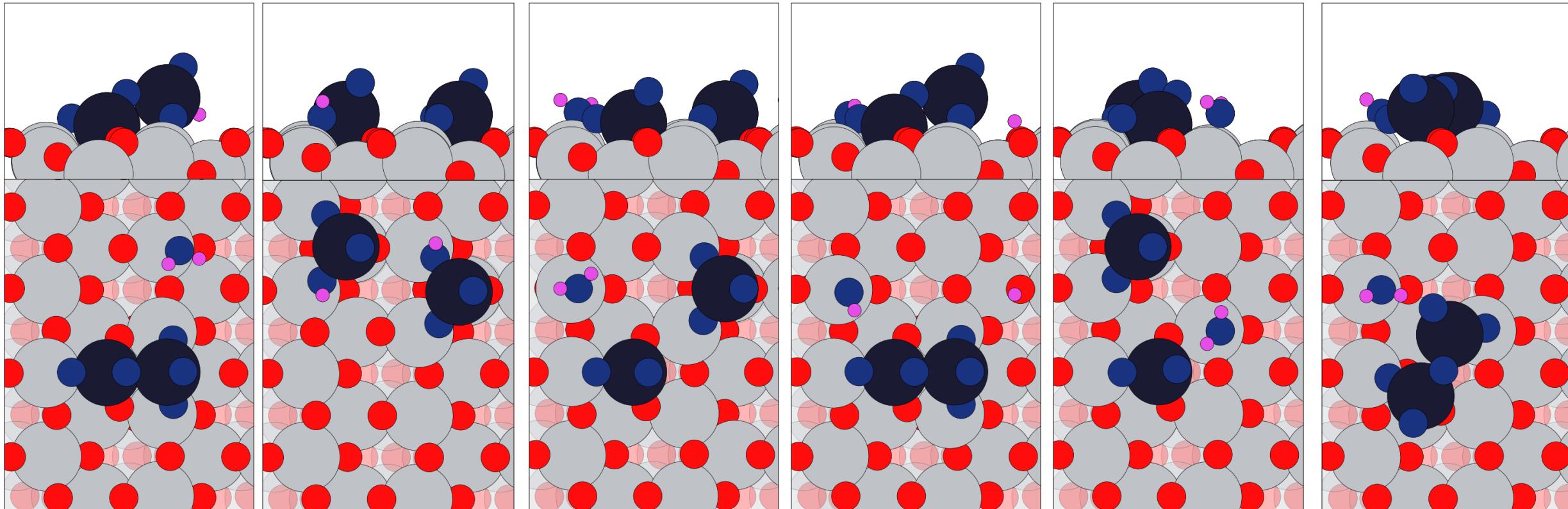
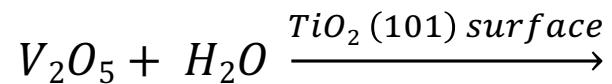
I8:  $\Delta E = 1.231 \text{ eV}$

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

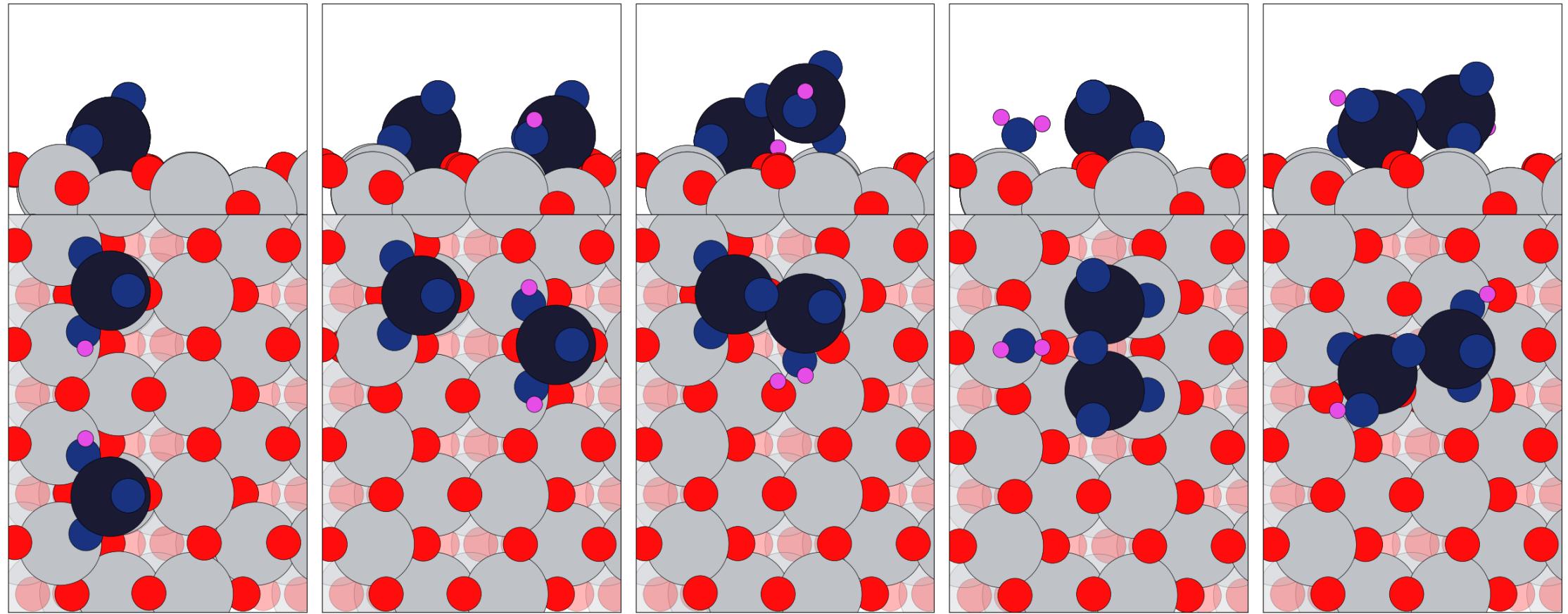
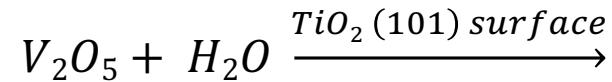
I3:  $\Delta E = 0.072 \text{ eV}$

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

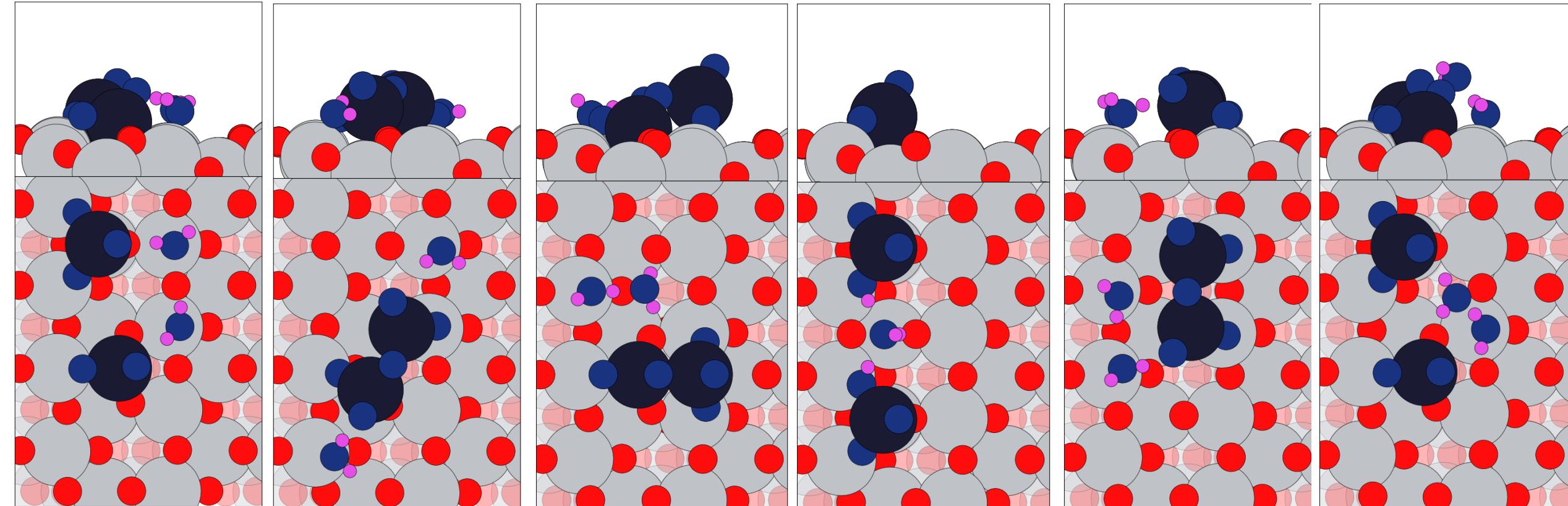
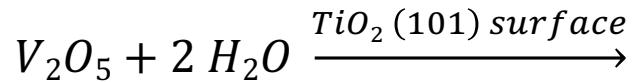
I8:  $\Delta E = 0.287 \text{ eV}$

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

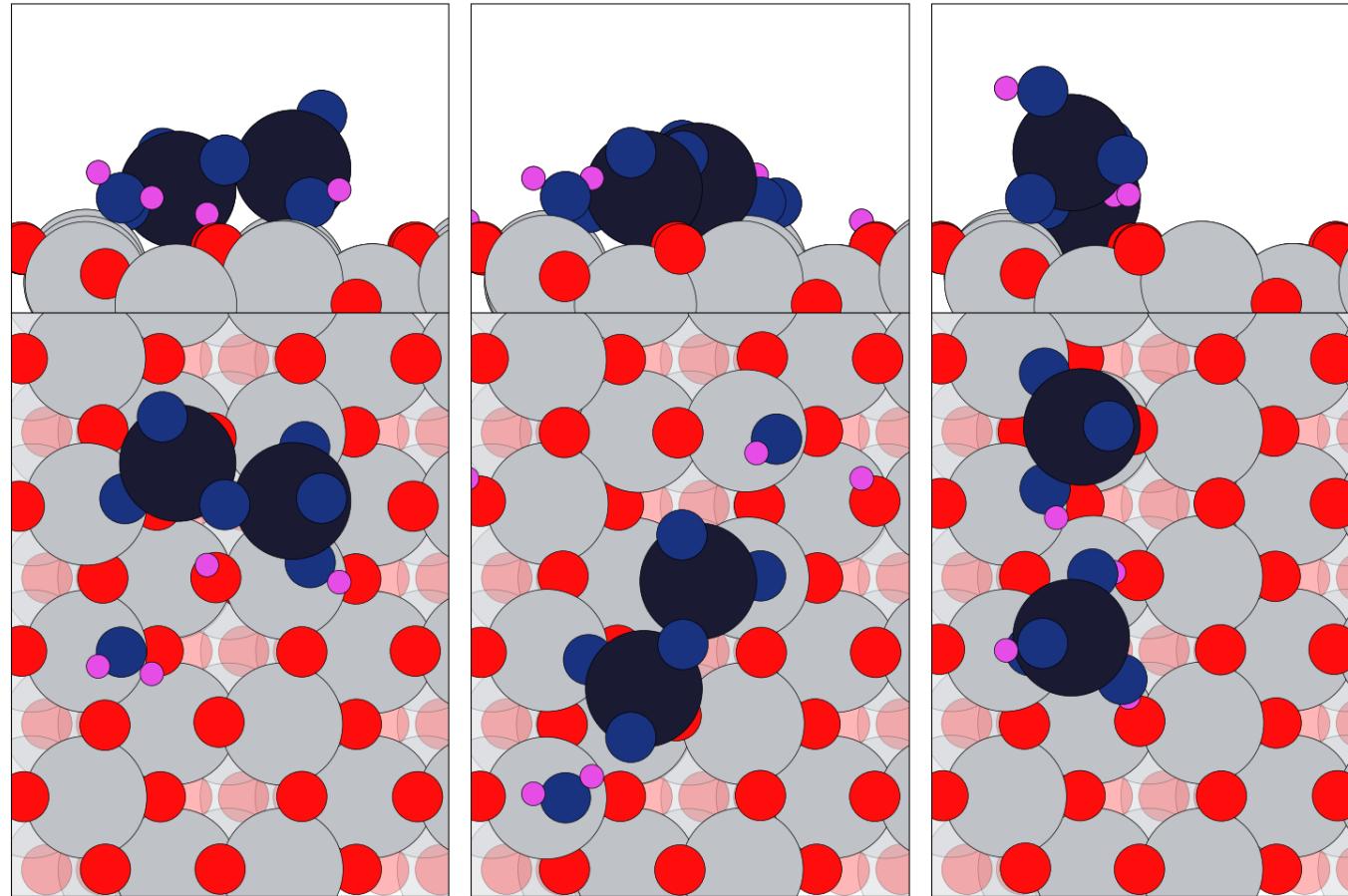
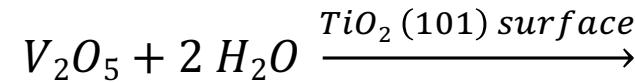
I3:  $\Delta E = 0.196 \text{ eV}$

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)

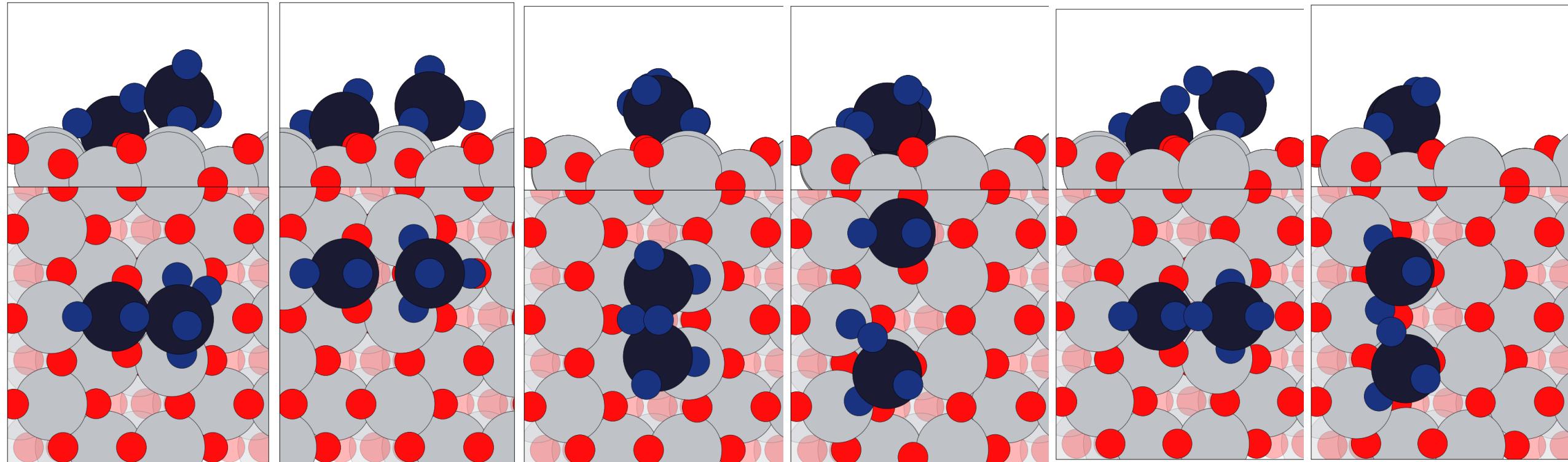


I7:  $\Delta E = 0.399 \text{ eV}$

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

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

# $\text{V}_2\text{O}_6$ Clusters (1by3 Super cell)



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

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

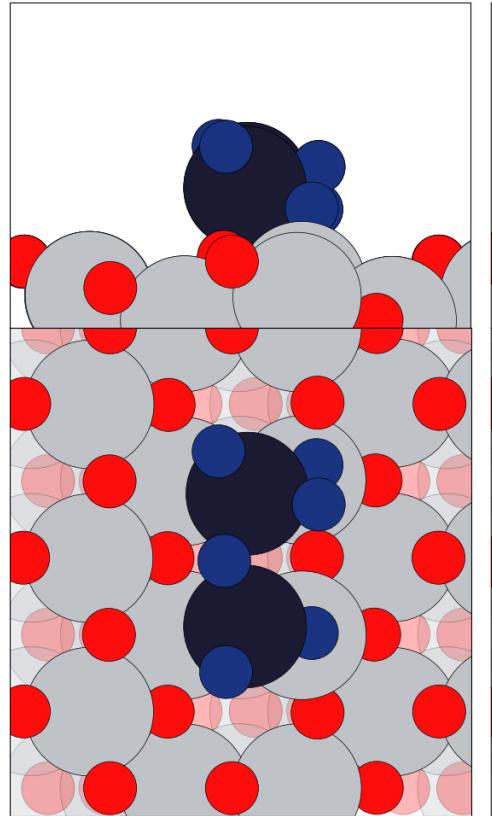
I3:  $\Delta E = 0.254 \text{ eV}$

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

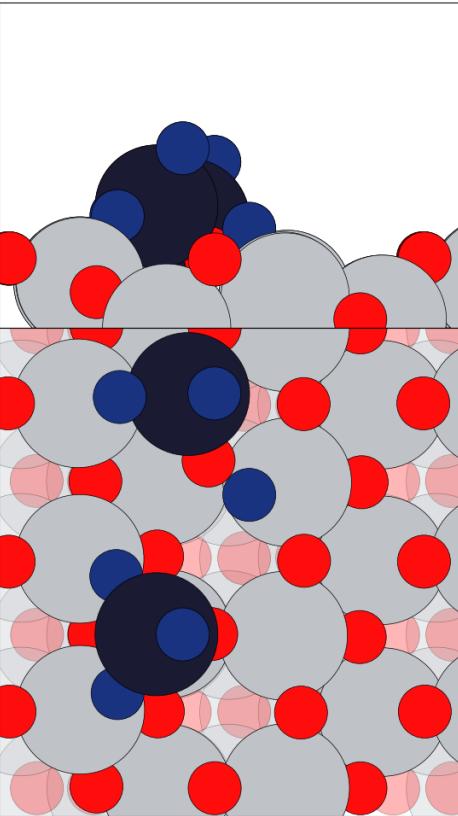
I5:  $\Delta E = 0.388 \text{ eV}$

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

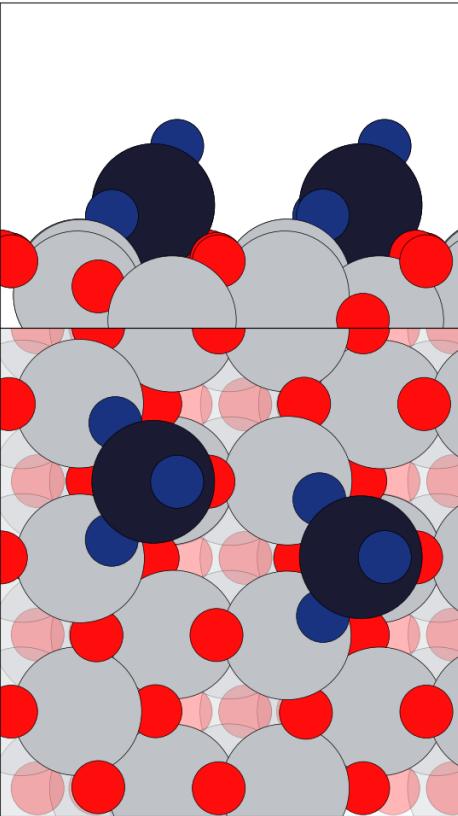
# $\text{V}_2\text{O}_6$ Clusters (1by3 Super cell)



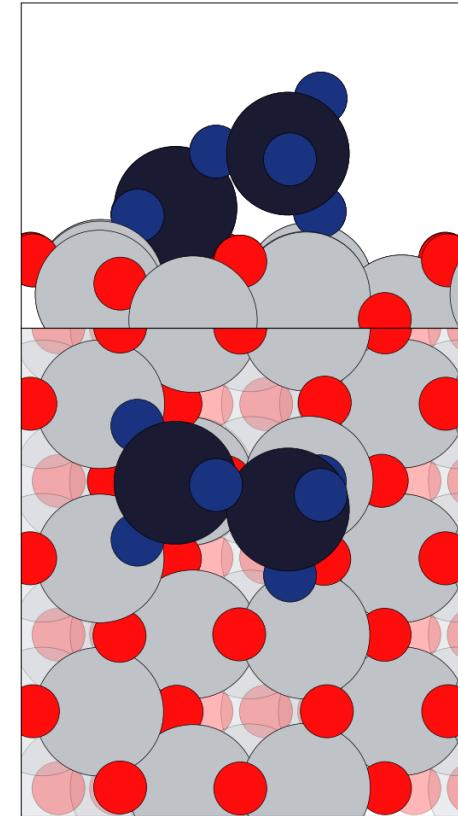
I7:  $\Delta E = 0.479 \text{ eV}$



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

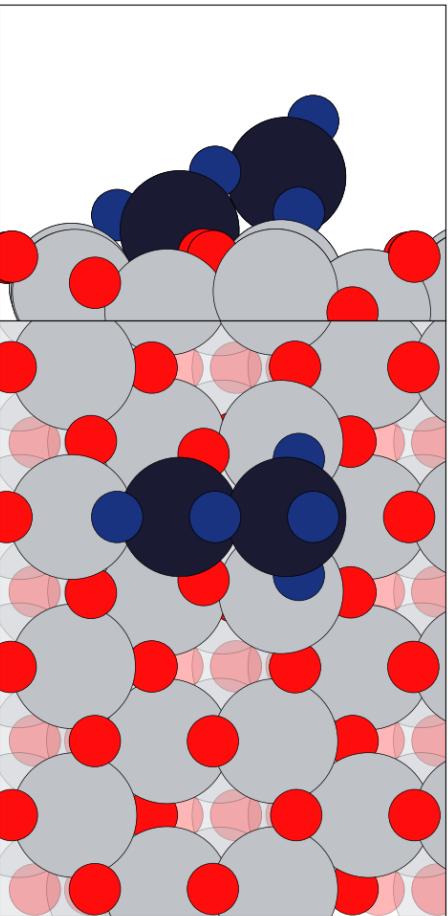


I9:  $\Delta E = 1.373 \text{ eV}$



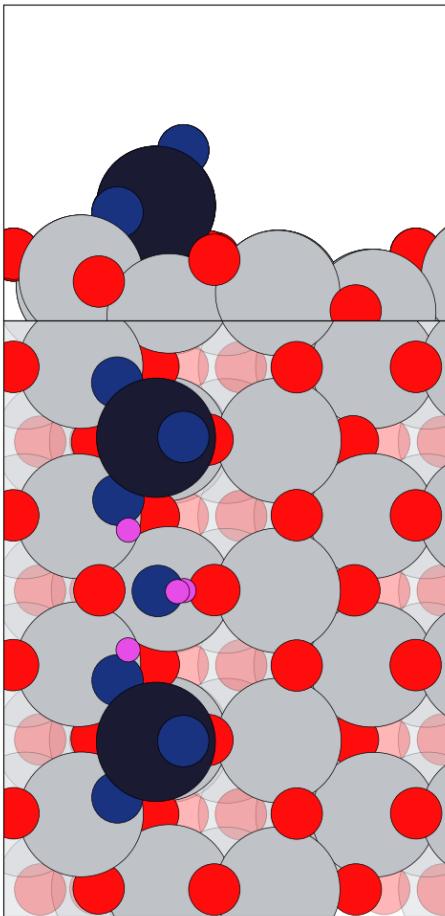
I10:  $\Delta E = 1.912 \text{ eV}$

Before H<sub>2</sub>O exposer



Global minimum

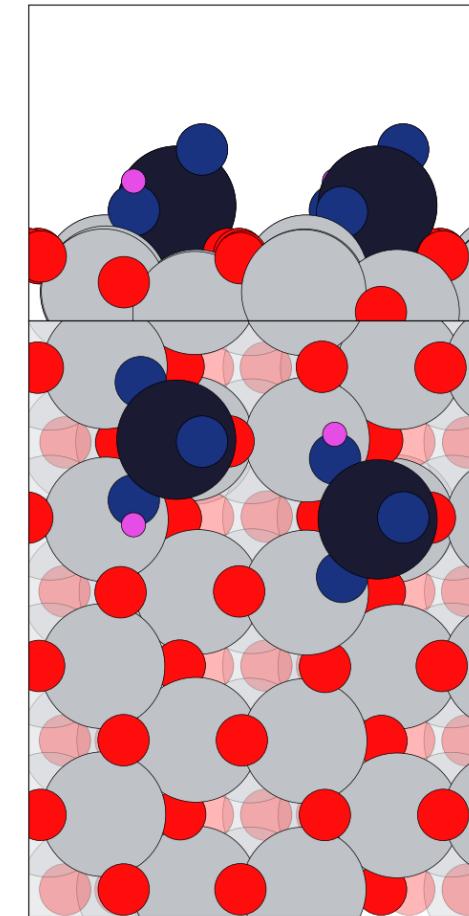
During H<sub>2</sub>O exposer



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

This becomes GM if we have  
more than 2 H<sub>2</sub>O

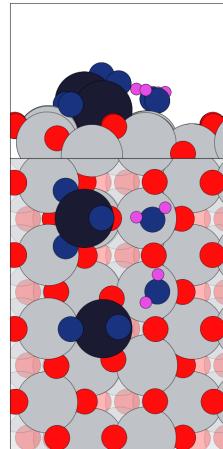
After H<sub>2</sub>O exposer



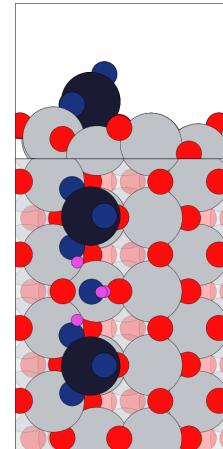
Global minimum

$U_{\text{eff}}$ (eV)	Stoichiometric surface $\Delta E$ (eV) $U_{\text{eff}}$ for only V	Reduced surface $\Delta E$ (eV) $U_{\text{eff}}$ for both V & Ti	Reduced surface $\Delta E$ (eV) $U_{\text{eff}}$ for only Ti	Stoichiometric surface $\Delta E$ (eV) $U_{\text{eff}}$ 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

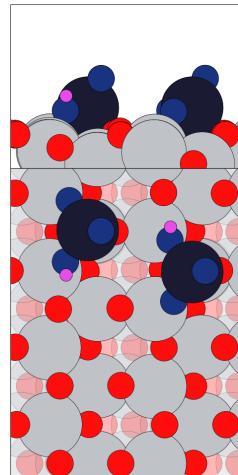


$$\Delta E = EI_2 - EI_1$$

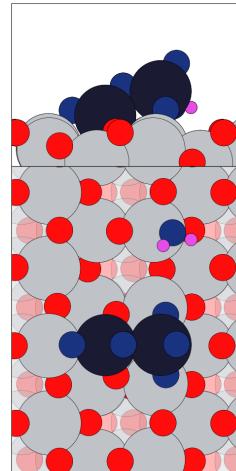
$$\Delta E = EI_2 - EI_1$$

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

I1



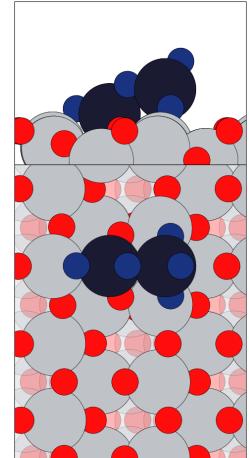
I2



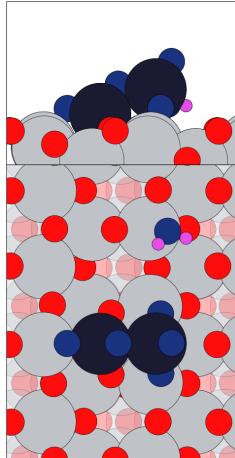
# Adsorption Energies By addition of H<sub>2</sub>O Molecule

E<sub>1</sub><sup>Ads</sup>

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

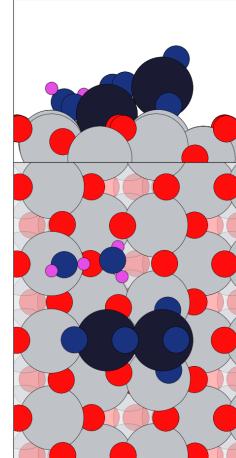


H<sub>2</sub>O →



ΔE = 0.076 eV

H<sub>2</sub>O →

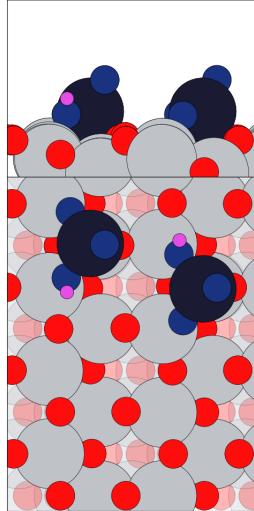


ΔE = 0.271 eV

	E <sub>ads</sub> (1 H <sub>2</sub> O) (eV)	E <sub>ads</sub> (2 H <sub>2</sub> O) (eV)	E <sub>ads</sub> (3 H <sub>2</sub> O) (eV)	E <sub>ads</sub> (5 H <sub>2</sub> O) (eV)
E <sub>1</sub> <sup>Ads</sup>	-0.871	1.546		
E <sub>2</sub> <sup>Ads</sup>	-1.264			
E <sub>3</sub> <sup>Ads</sup>	-1.013			
E <sub>4</sub> <sup>Ads</sup>	-0.912	-1.945	-2.929	-3.943
E <sub>5</sub> <sup>Ads</sup>	-1.982	-2.875	-3.694	-4.838

E<sub>2</sub><sup>Ads</sup>

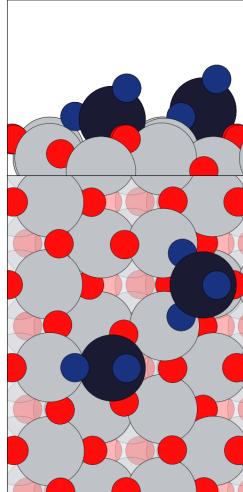
H<sub>2</sub>O →



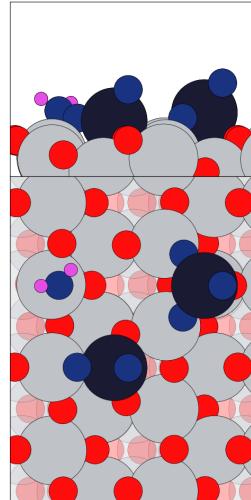
ΔE = 0.000 eV

E<sub>3</sub><sup>Ads</sup>

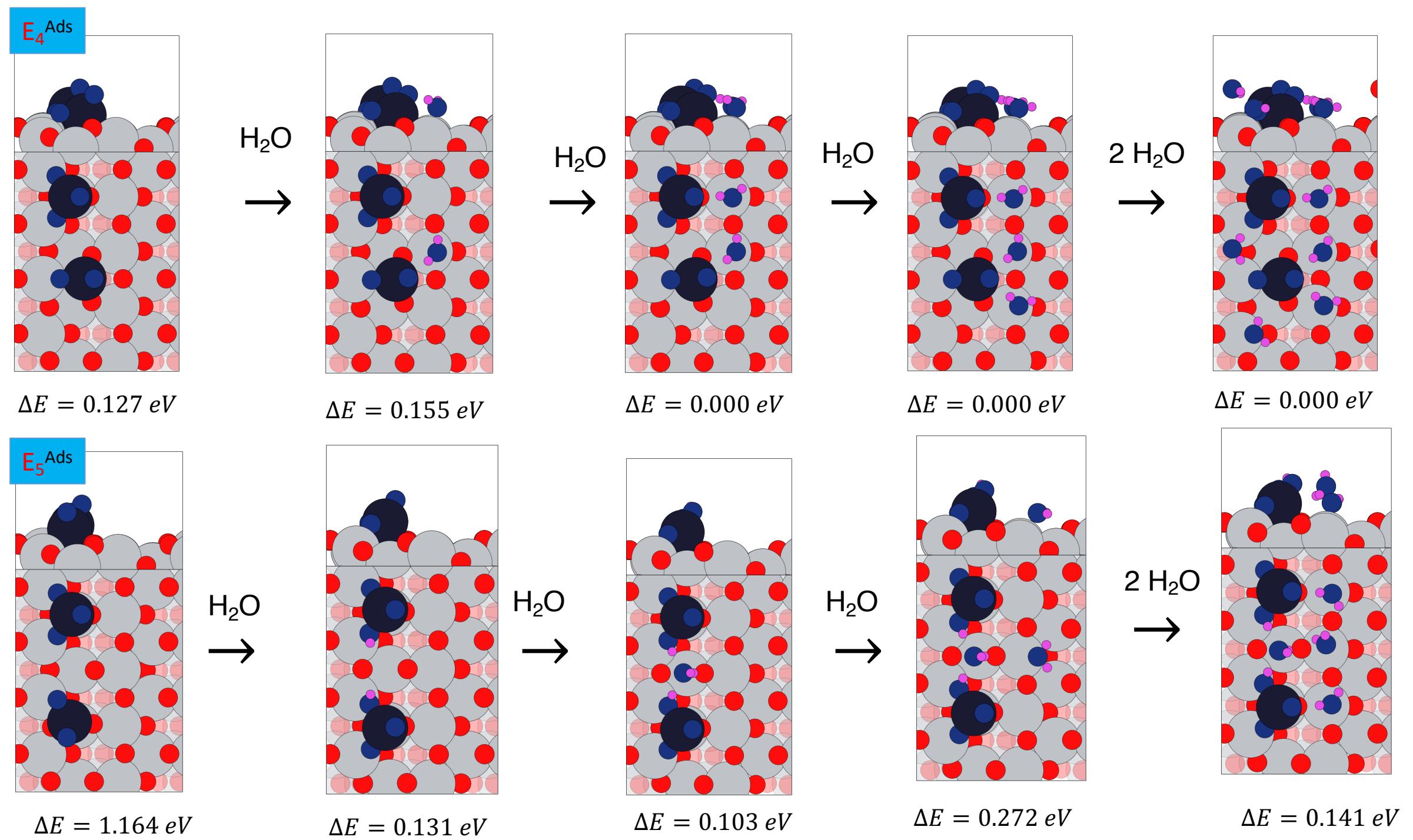
H<sub>2</sub>O →



ΔE = 0.131 eV



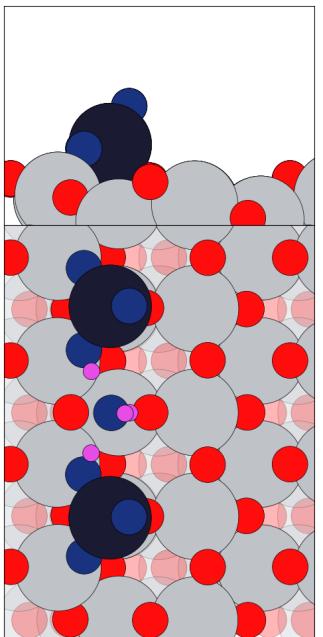
ΔE = 0.066 eV



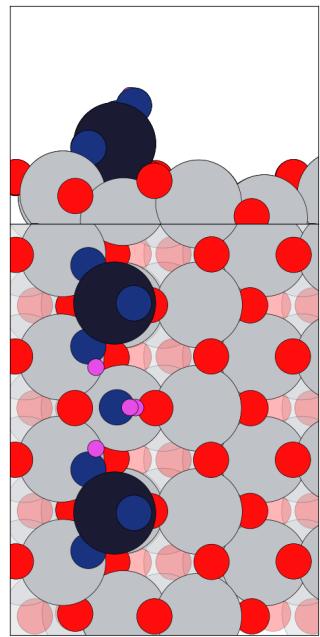
# Observations

## 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  
→



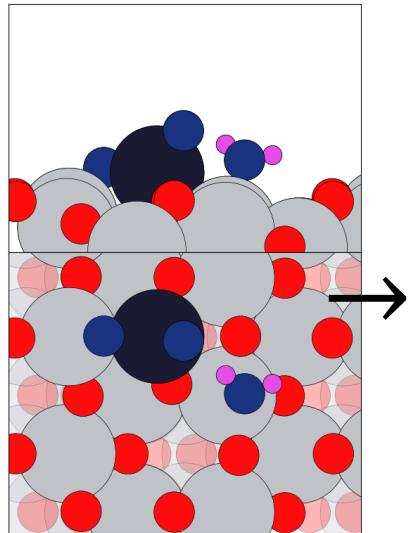
I4:  $\Delta E = 0.254 \text{ eV}$

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

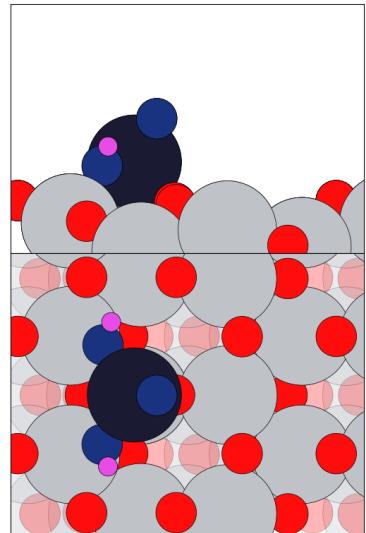
# Observations

## 2) Dissociation capability of H<sub>2</sub>O due to size of Cluster:

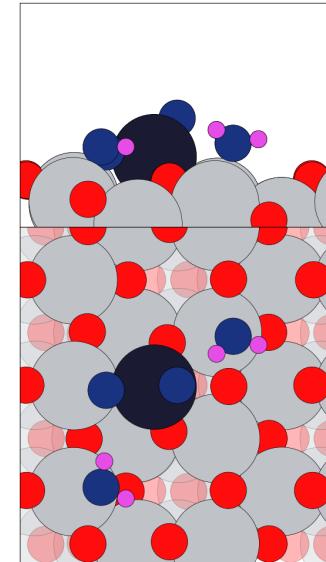
In case of VO<sub>2</sub> cluster, it requires 0.131 eV/1 H<sub>2</sub>O and 0.053 eV/2 H<sub>2</sub>O energy to dissociate the H<sub>2</sub>O. And In case of V<sub>2</sub>O<sub>4</sub> and V<sub>2</sub>O<sub>5</sub>, dissociated H<sub>2</sub>O strcture is the GM.



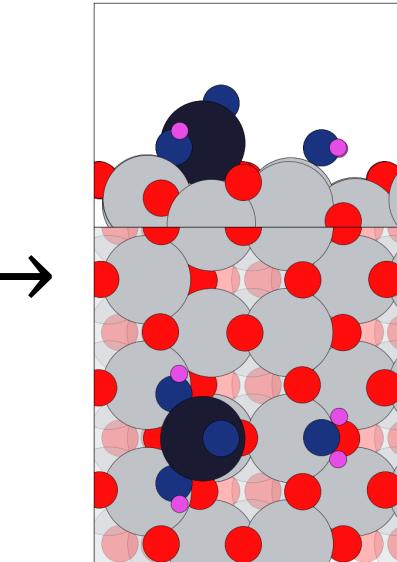
I1:  $\Delta E = 0.000 \text{ eV}$



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



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

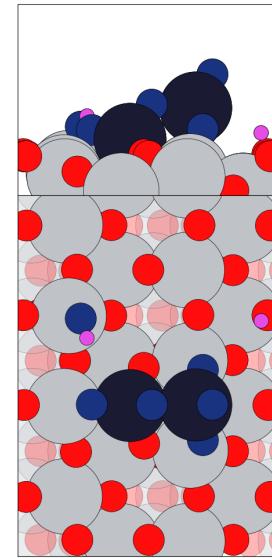
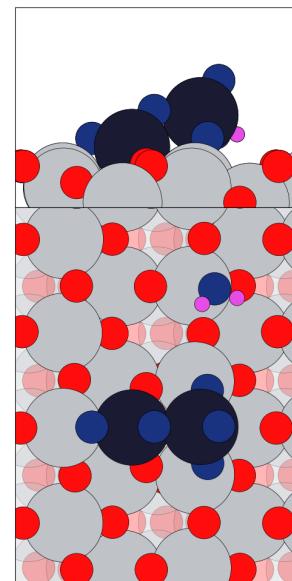
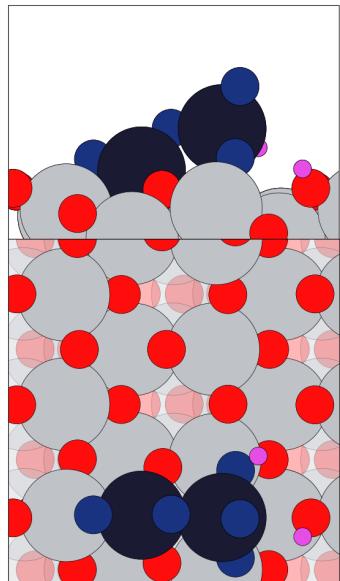
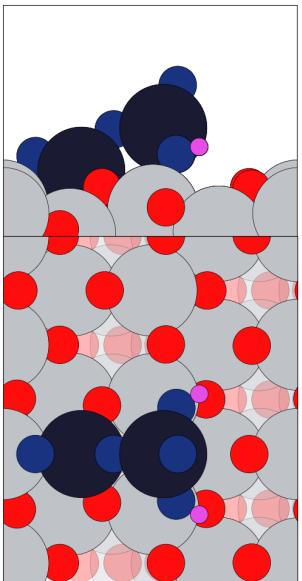


I3:  $\Delta E = 0.053 \text{ eV}$

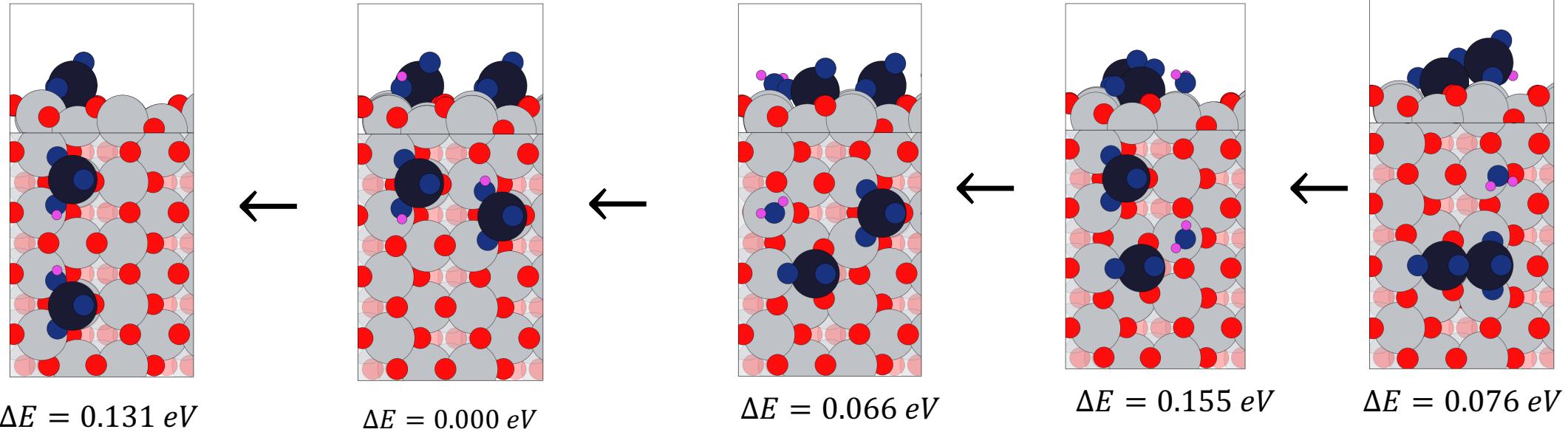
# Observations

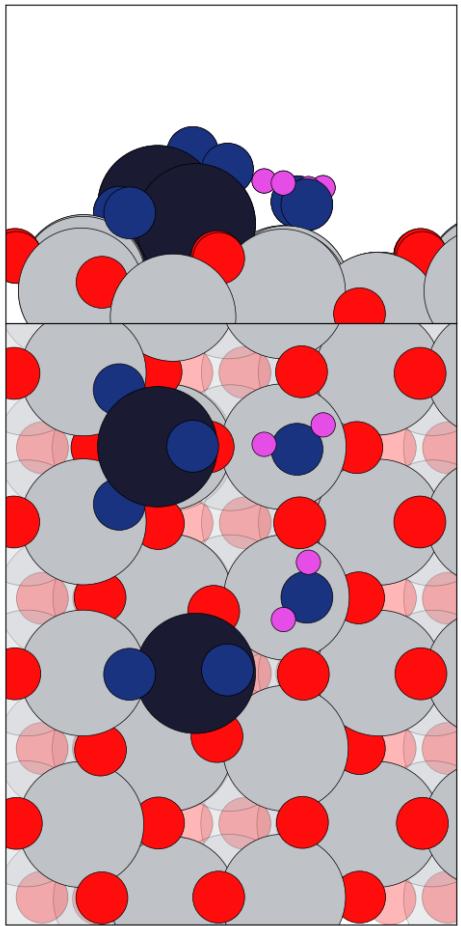
## 3) Surface Effect on H<sub>2</sub>O dissociation:

We did not observed the surface hydroxyls within 0.2 eV energy range from GM. Mostly Vanadium oxide clusters are responsible for H<sub>2</sub>O dissociation.

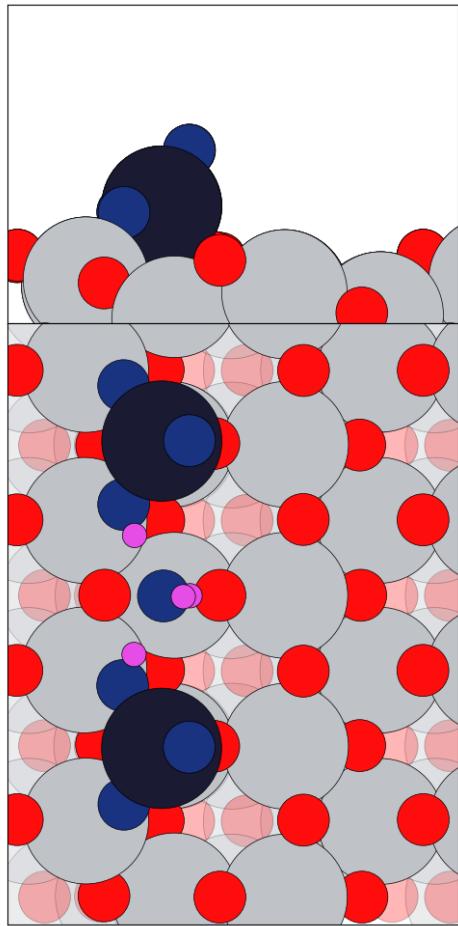


# Adsorption Energy order

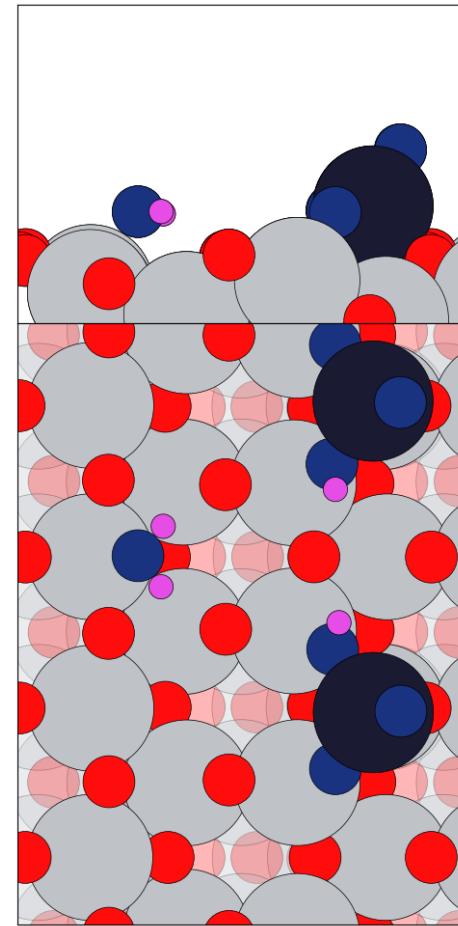




$$\Delta E = 0.000 \text{ eV}$$

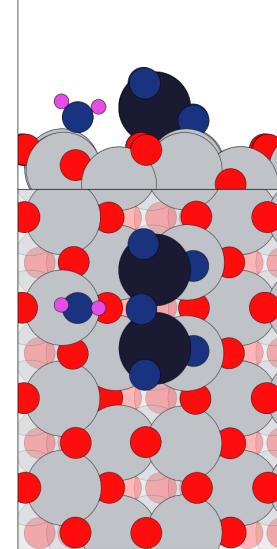
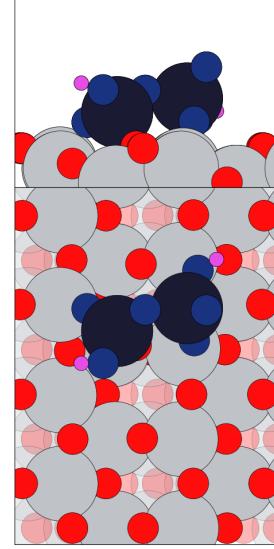
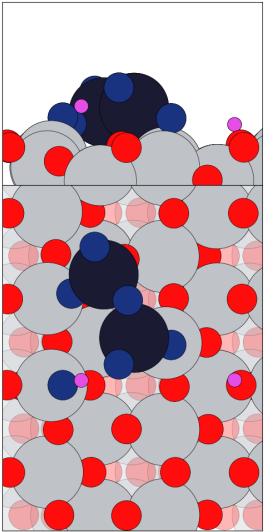
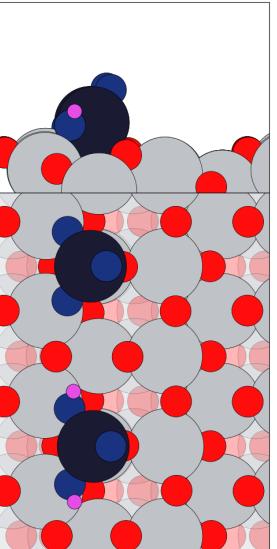
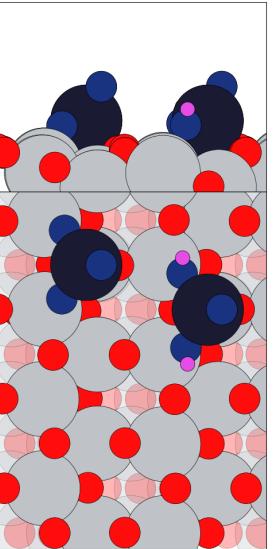
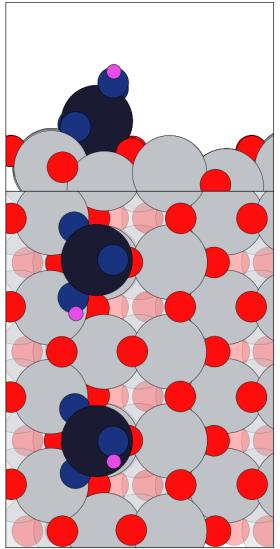


$$\Delta E = 0.08 \text{ eV}$$



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

# Binding Energy of H<sub>2</sub>O for V<sub>2</sub>O<sub>5</sub>+H<sub>2</sub>O (O<sub>v</sub>+csr)



I9:E<sub>bind</sub> = -0.767 eV

I10:E<sub>bind</sub> = -0.717 eV

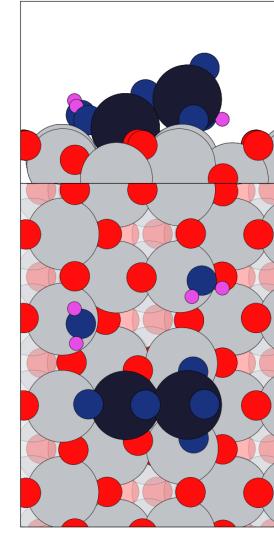
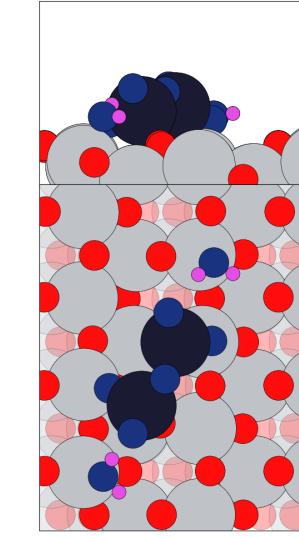
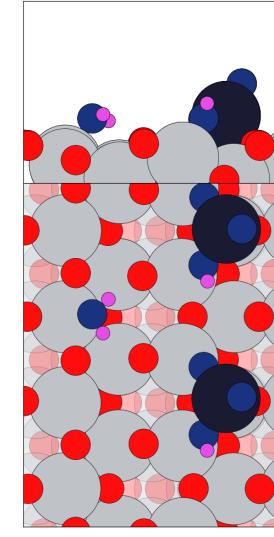
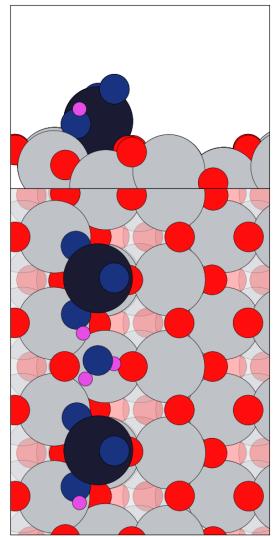
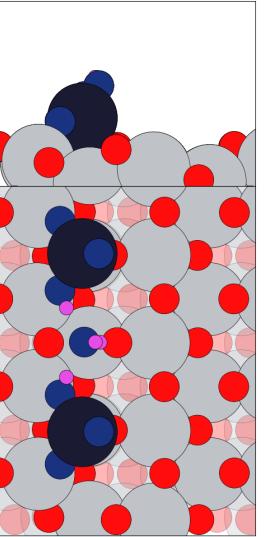
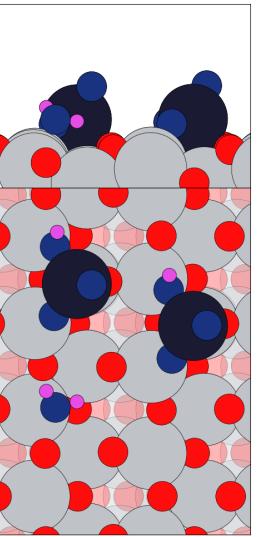
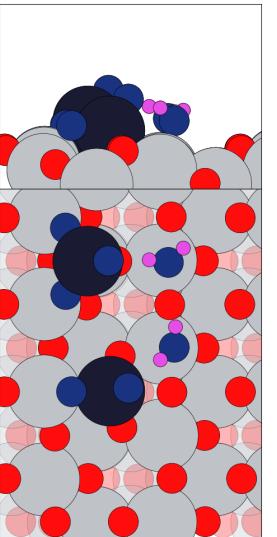
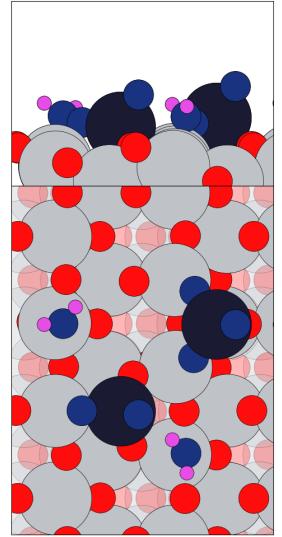
I11:E<sub>bind</sub> = -0.609 eV

I12:E<sub>bind</sub> = -0.550 eV

I13:E<sub>bind</sub> = -0.465 eV

I14:E<sub>bind</sub> = -0.428 eV

# Binding Energy of H<sub>2</sub>O for V<sub>2</sub>O<sub>5</sub>+2 H<sub>2</sub>O (O<sub>v</sub>+csr)



I1:E<sub>bind</sub> = -1.864 eV

I1:E<sub>bind</sub> = -1.816 eV

I1:E<sub>bind</sub> = -1.809 eV

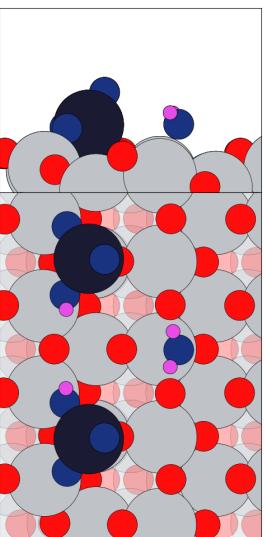
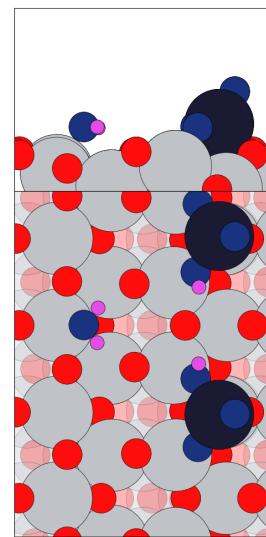
I2:E<sub>bind</sub> = -1.710 eV

I3:E<sub>bind</sub> = -1.698 eV

I3:E<sub>bind</sub> = -1.693 eV

I4:E<sub>bind</sub> = -1.646 eV

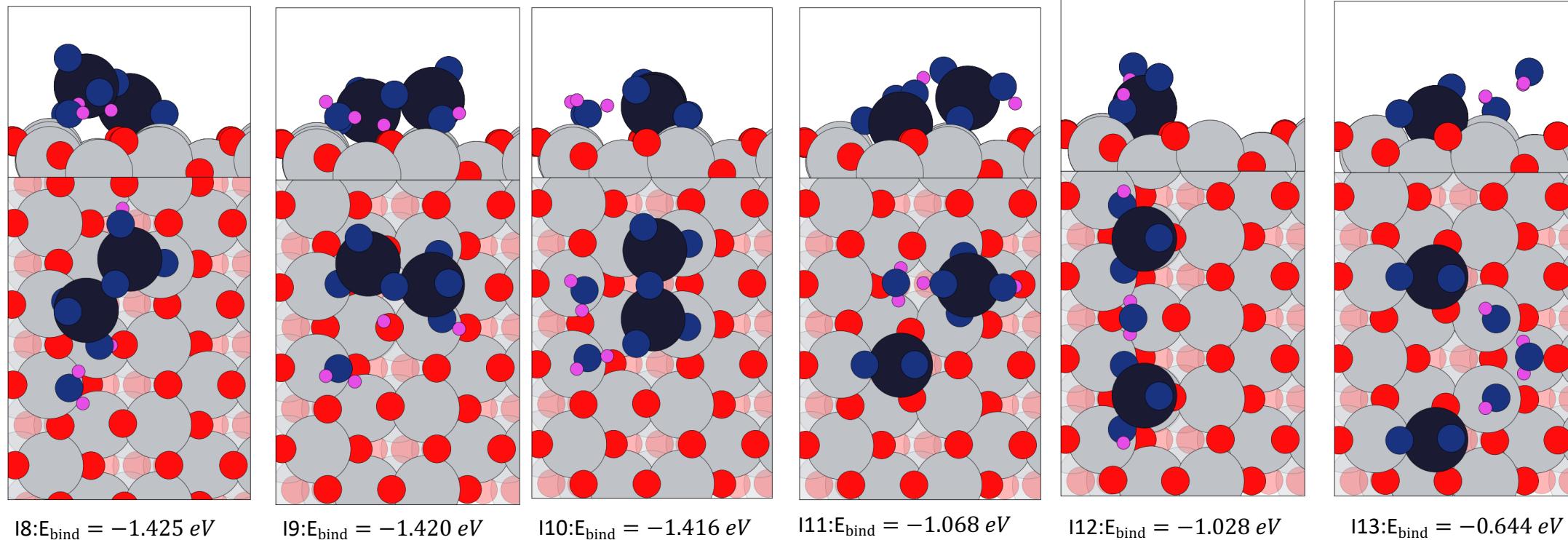
I6:E<sub>bind</sub> = -1.637 eV

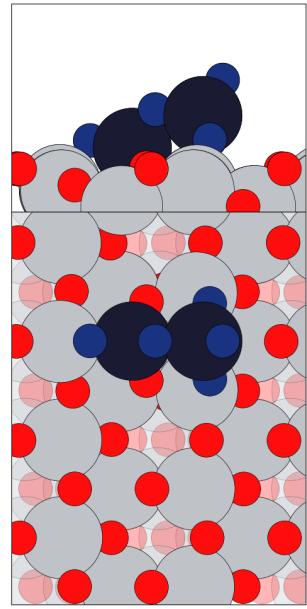


I5:E<sub>bind</sub> = -1.632 eV

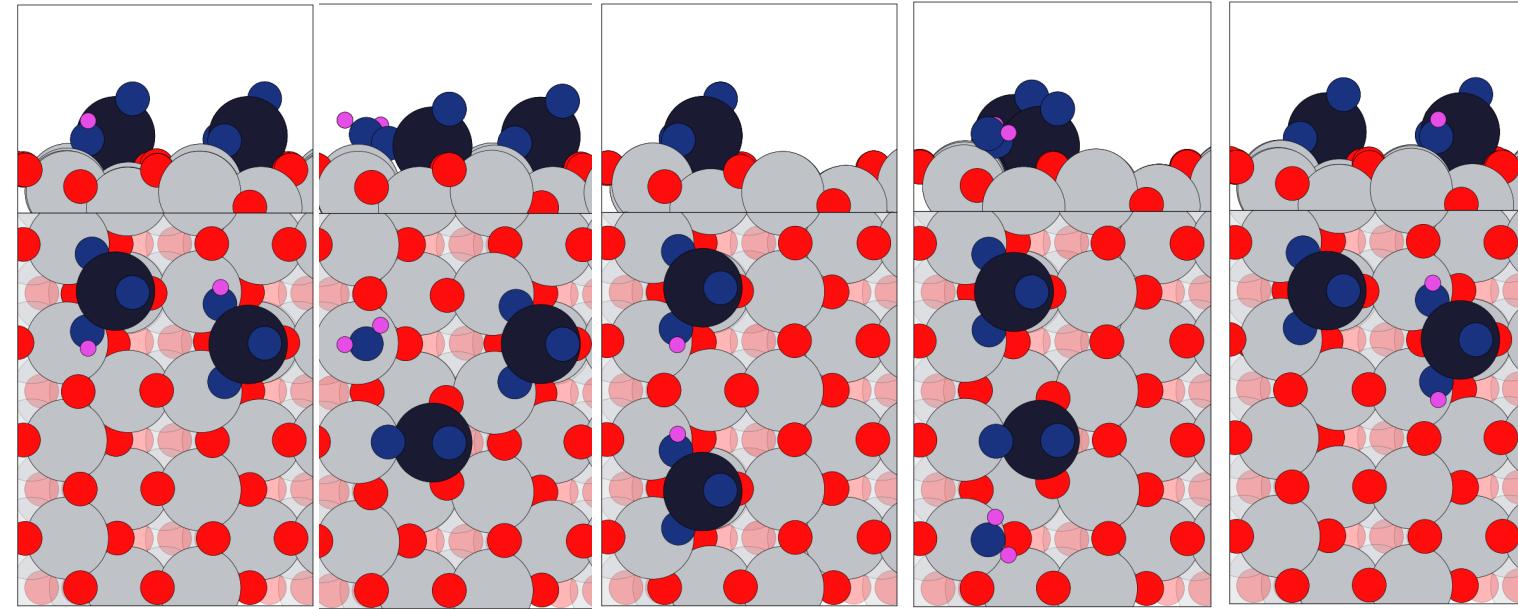
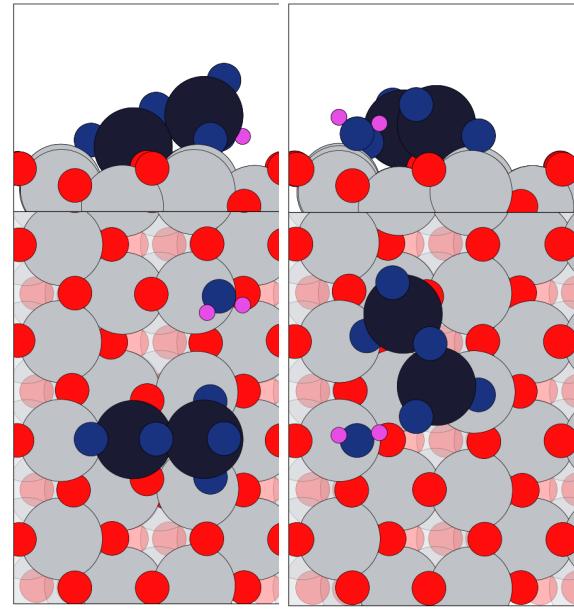
I7:E<sub>bind</sub> = -1.438 eV

# Binding Energy of H<sub>2</sub>O for V<sub>2</sub>O<sub>5</sub>+2 H<sub>2</sub>O (O<sub>v</sub>+csr)

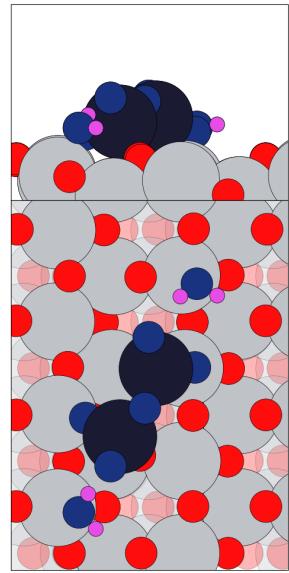




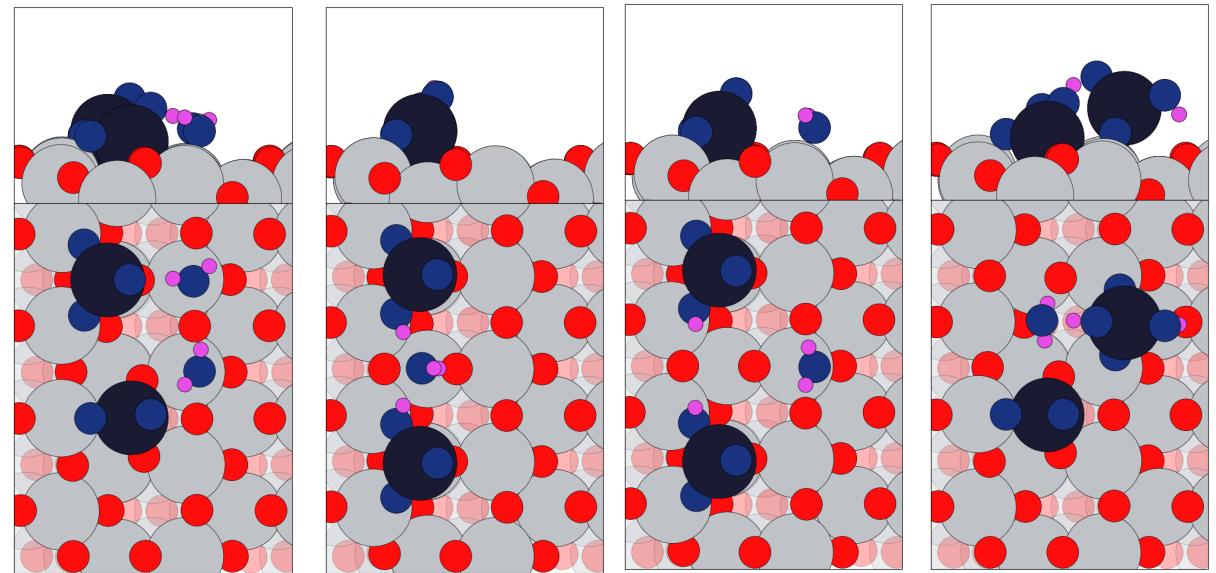
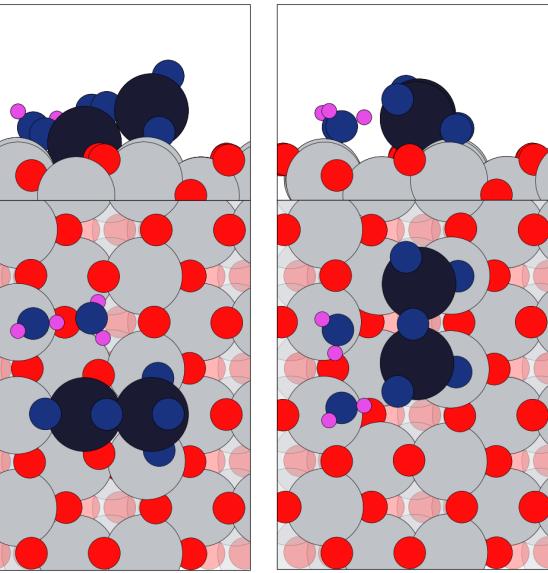
I3: $E_{\text{bind}} = -0.871 \text{ eV}$  I7: $E_{\text{bind}} = -0.780 \text{ eV}$



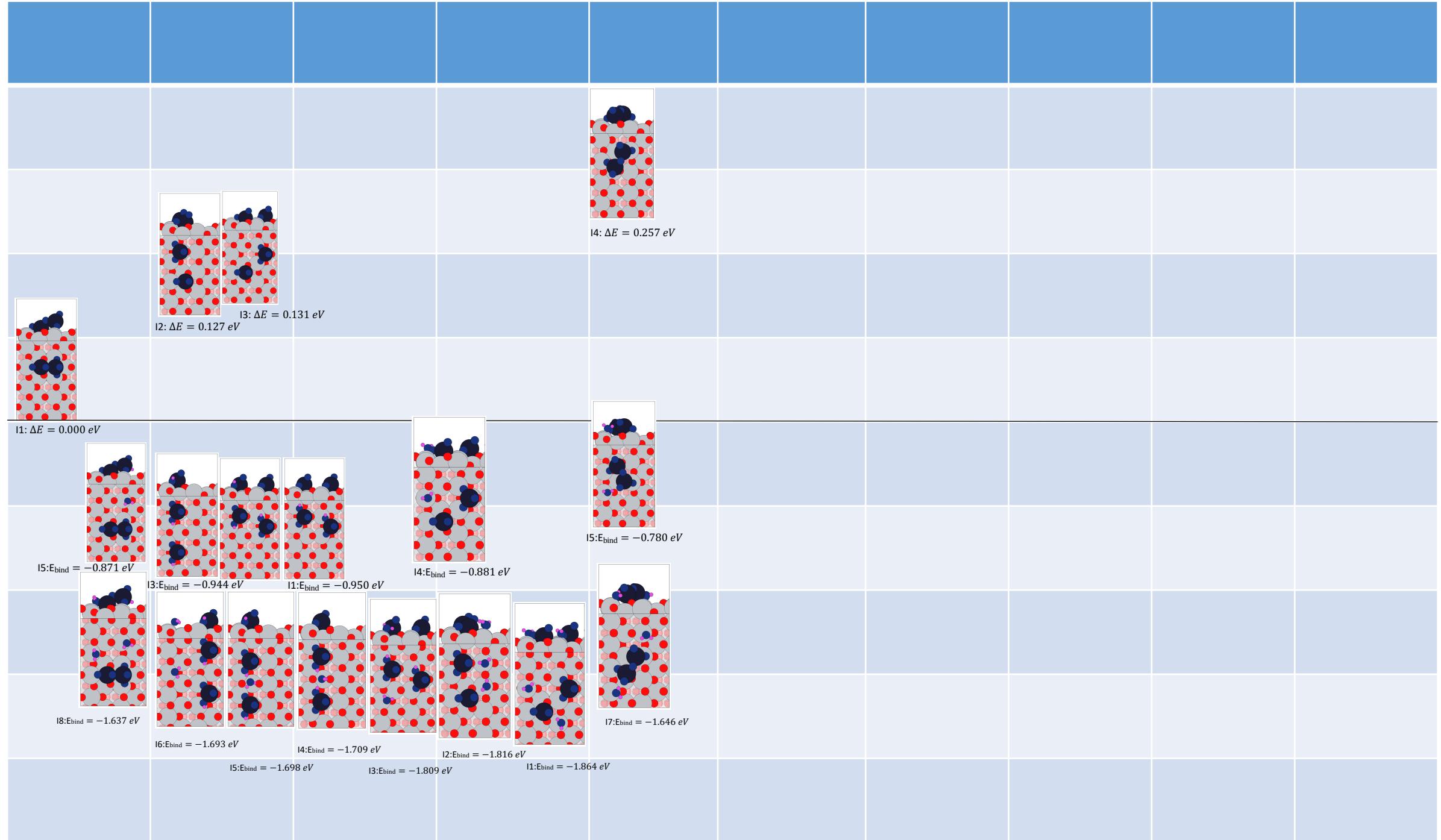
I1: $E_{\text{bind}} = -0.948 \text{ eV}$  I2: $E_{\text{bind}} = -0.881 \text{ eV}$  I5: $E_{\text{bind}} = -0.816 \text{ eV}$  I8: $E_{\text{bind}} = -0.751 \text{ eV}$  I9: $E_{\text{bind}} = -0.717 \text{ eV}$



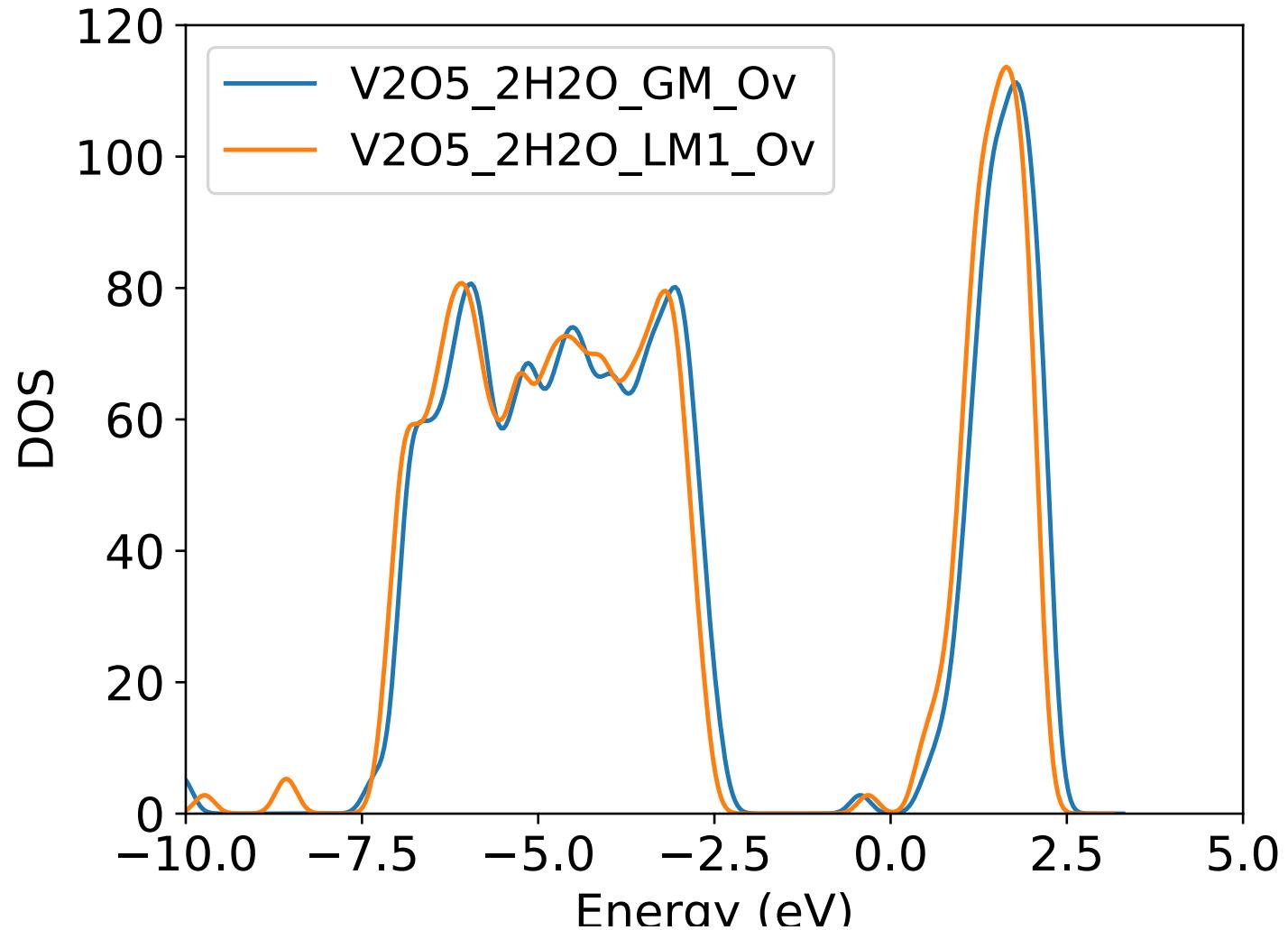
I3: $E_{\text{bind}} = -0.823 \text{ eV}$  I4: $E_{\text{bind}} = -0.773 \text{ eV}$  I7: $E_{\text{bind}} = -0.708 \text{ eV}$



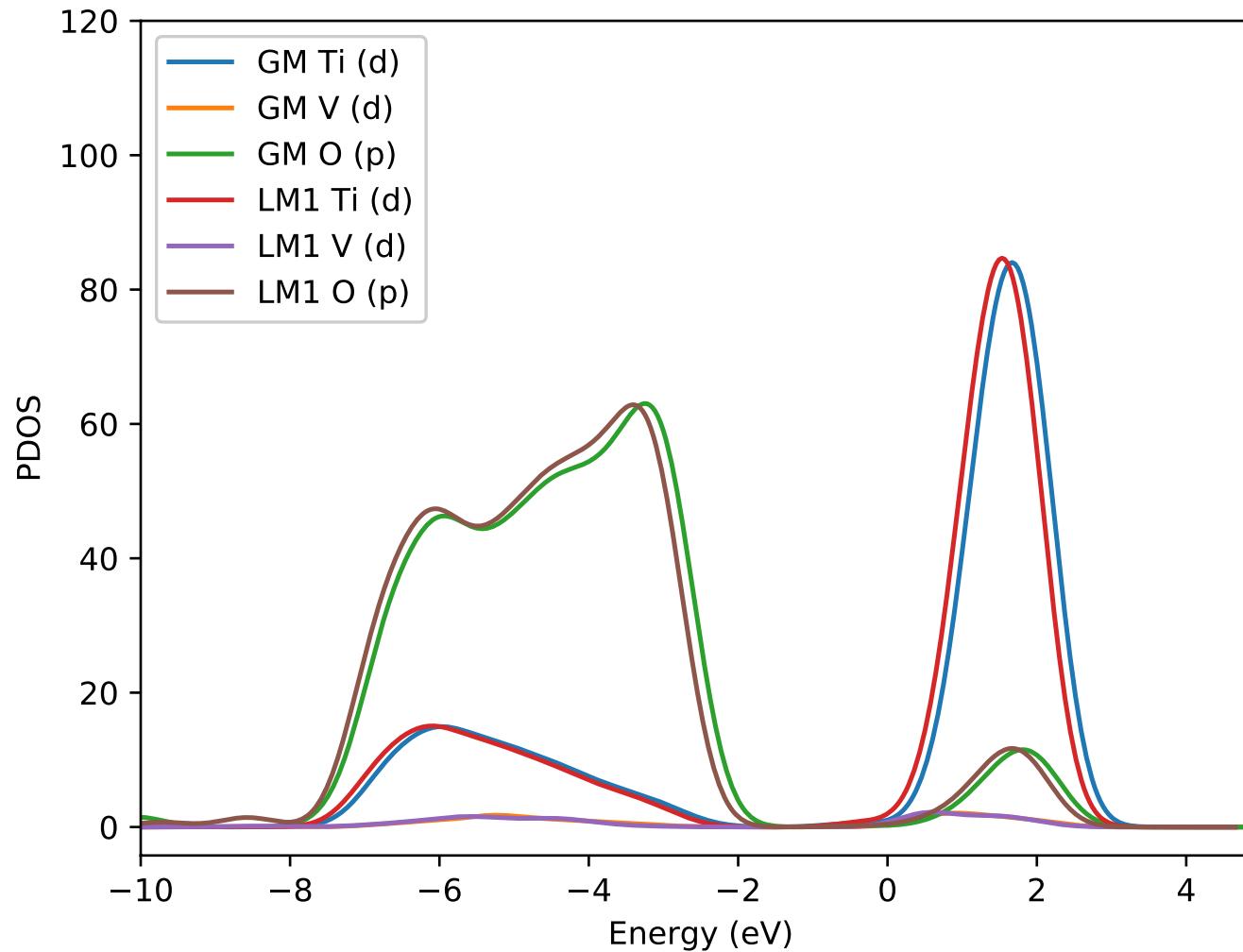
I1: $E_{\text{bind}} = -0.908 \text{ eV}$  I2: $E_{\text{bind}} = -0.855 \text{ eV}$  I5: $E_{\text{bind}} = -0.719 \text{ eV}$  I7: $E_{\text{bind}} = -0.534 \text{ eV}$

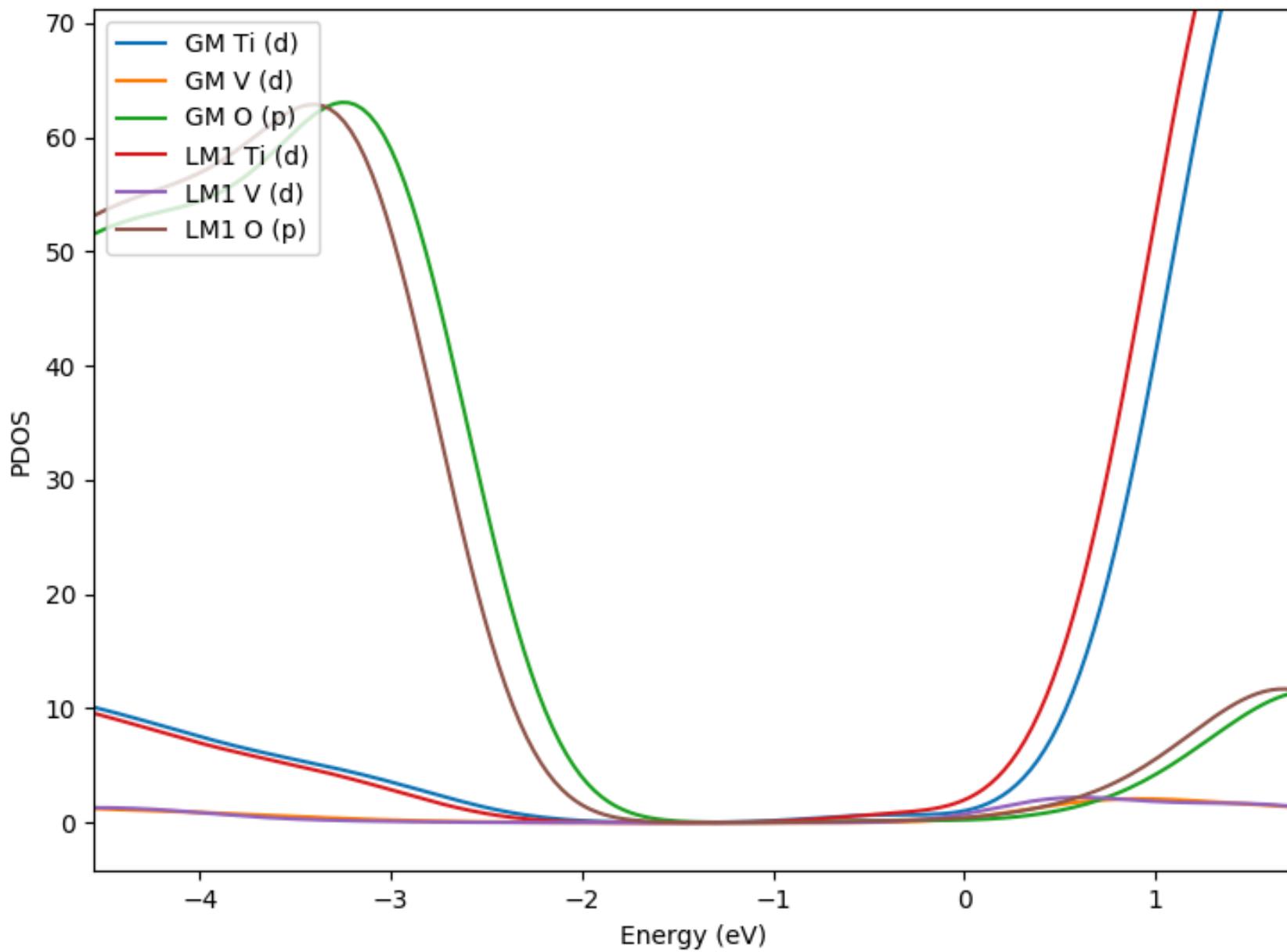


# Density of States



# Density of States





# Observations

## 4) Dissociation of V<sub>2</sub>O<sub>5</sub> clusters and Non-dissociation of V<sub>2</sub>O<sub>4</sub> clusters:

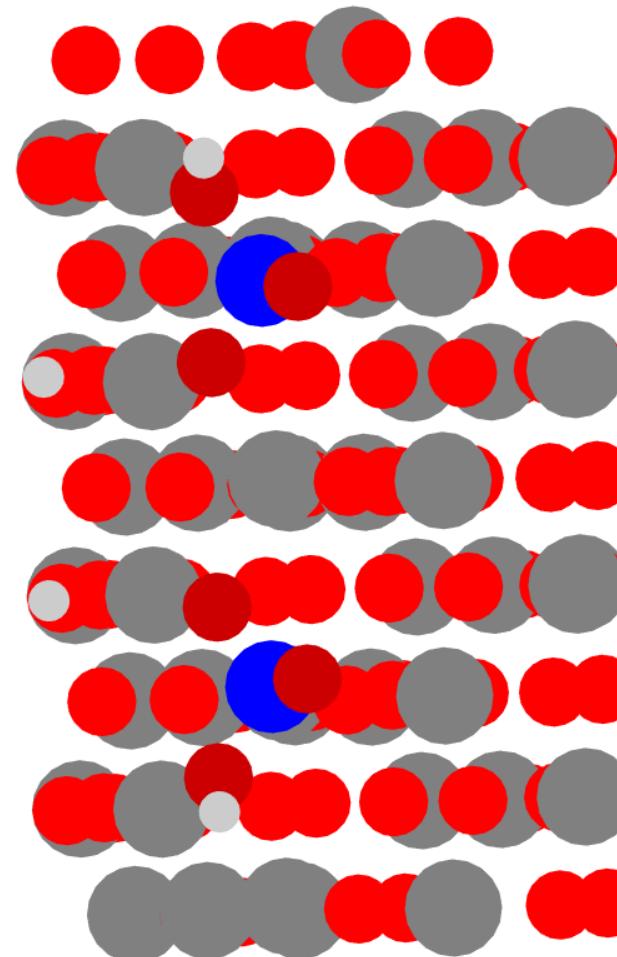
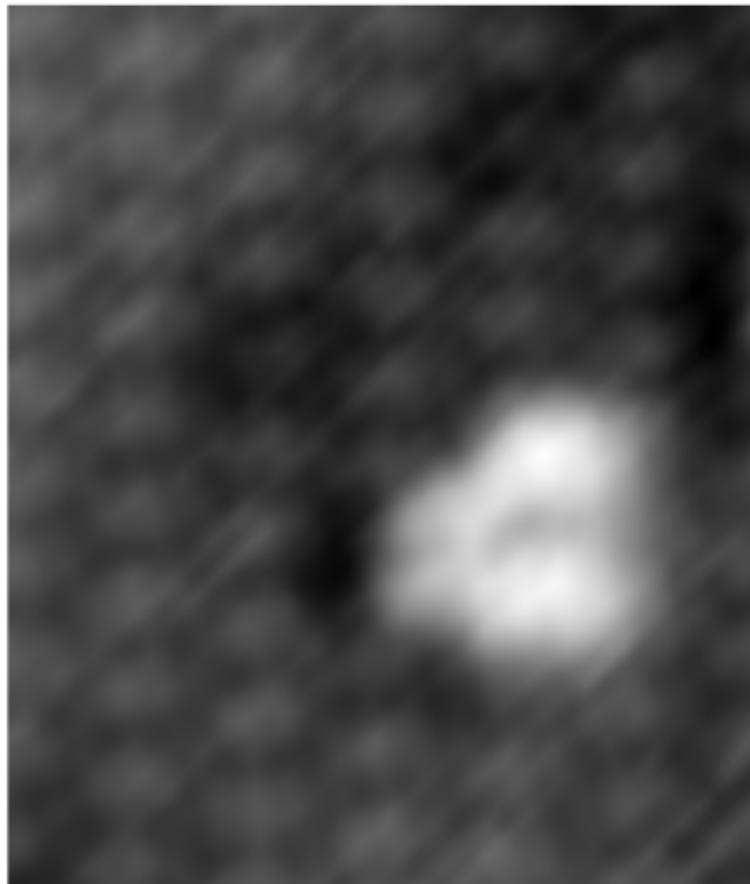
In case of V<sub>2</sub>O<sub>5</sub> clusters during H<sub>2</sub>O exposure, the cluster get dissociated in two paces (Ex: VO<sub>3</sub>H) and in case of V<sub>2</sub>O<sub>4</sub> during H<sub>2</sub>O exposure also the clusters get remains intact due to keeping of +4 or +5 state of Vanadium oxidation state.

## 5) Restructuring of V<sub>2</sub>O<sub>5</sub> cluster during H<sub>2</sub>O exposure:

The re-structuring of V<sub>2</sub>O<sub>5</sub> cluster during water exposure is due to dissociation of H<sub>2</sub>O makes the V<sub>2</sub>O<sub>5</sub> cluster in to two VO<sub>3</sub>H clusters and these two VO<sub>3</sub>H clusters can have different arrangements.

# Suggestions for a structure

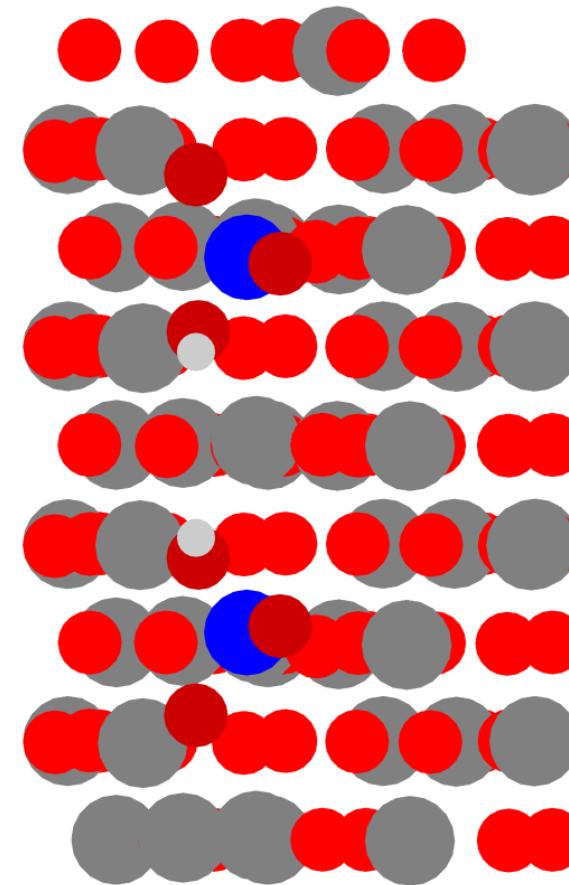
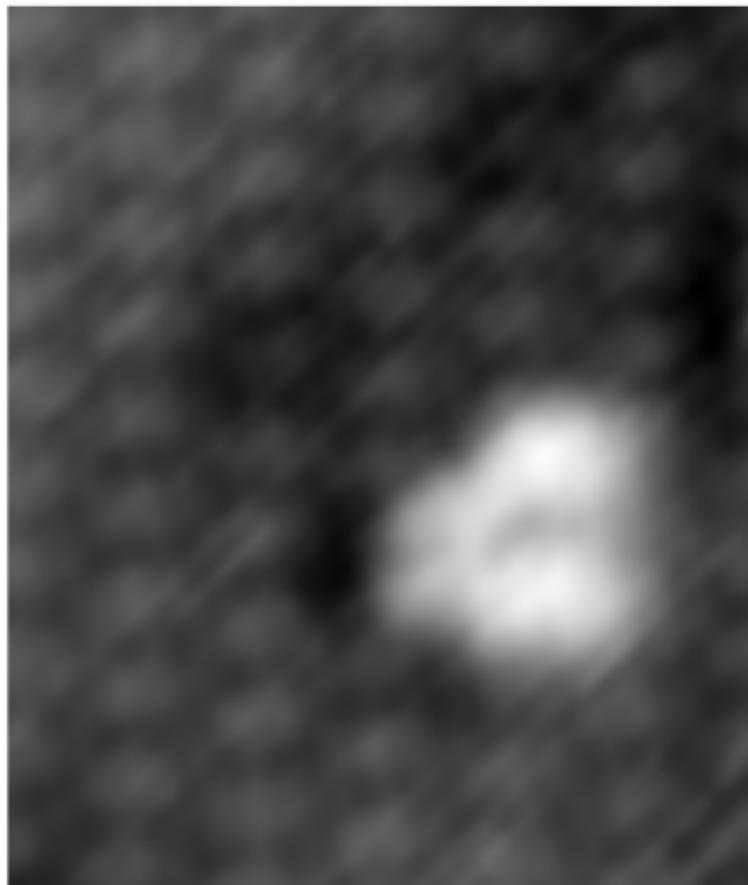
During Water exposure



2xV  
6xO  
4xH

# Suggestions for a structure

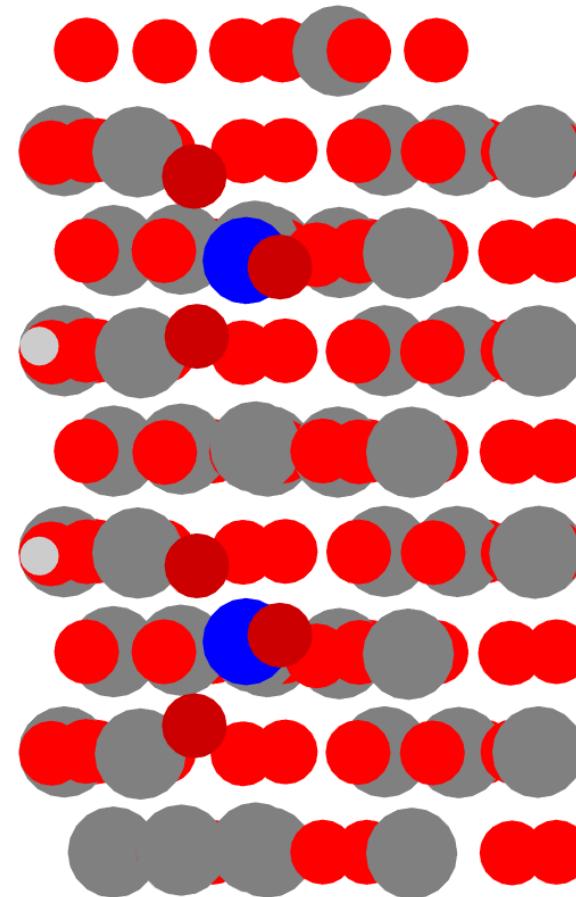
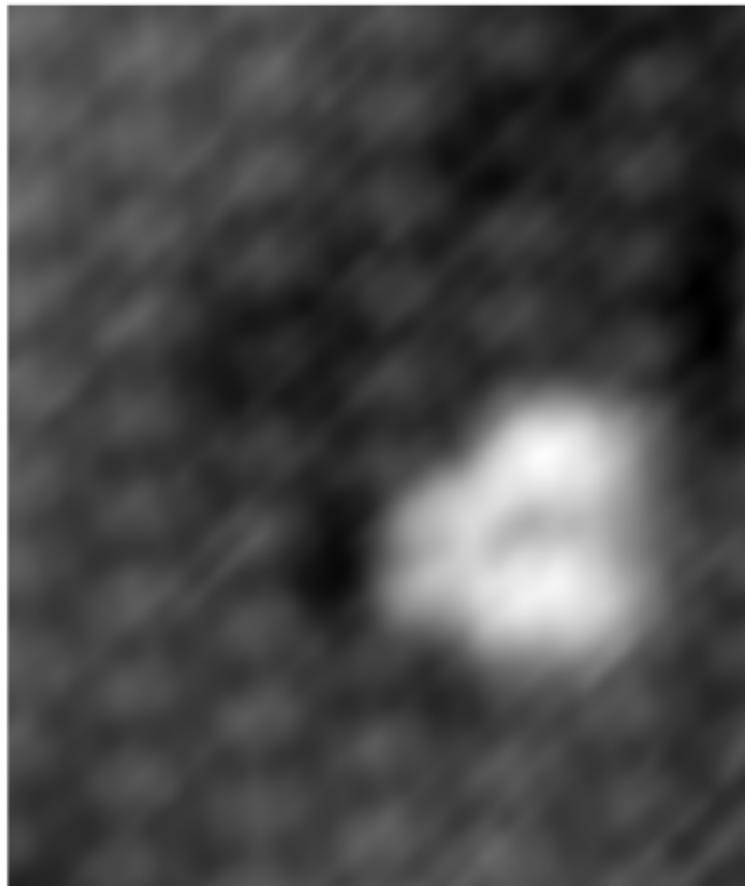
During Water exposure



2xV  
6XO  
2XH

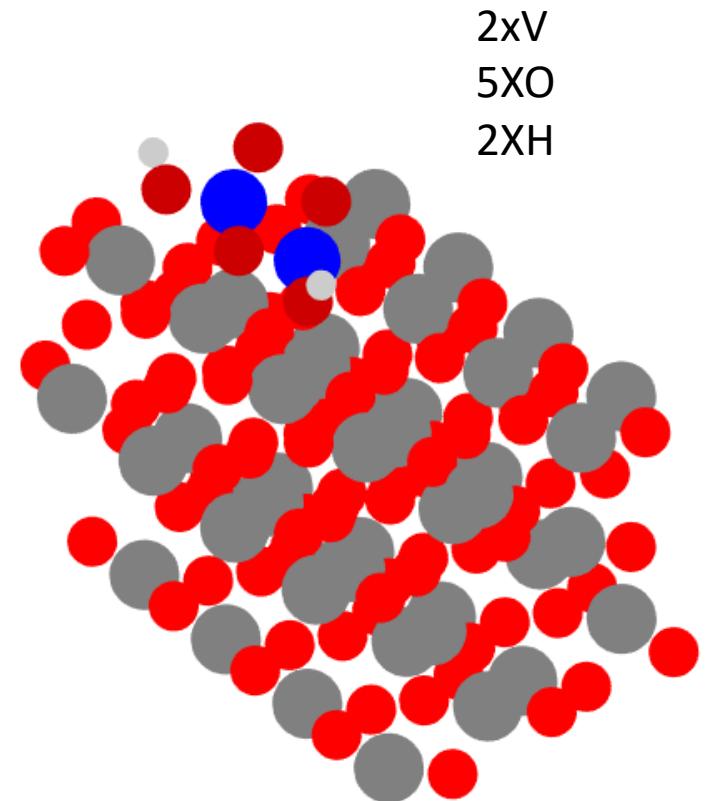
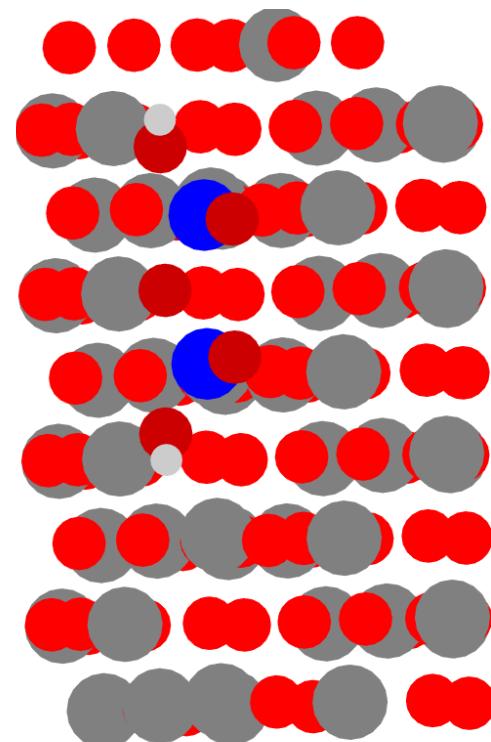
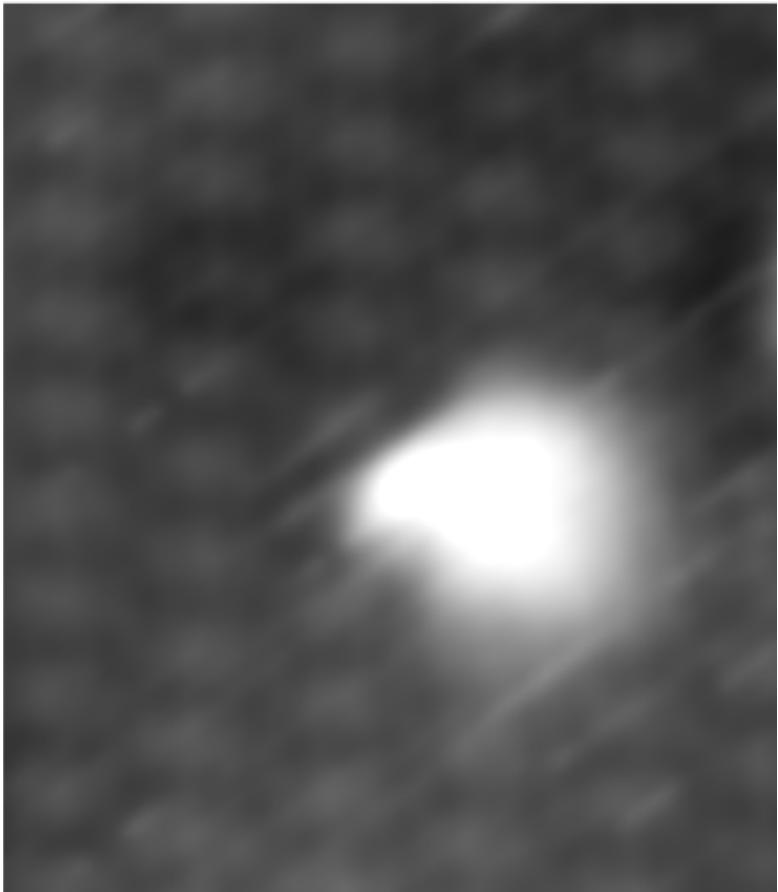
# Suggestions for a structure

During Water exposure



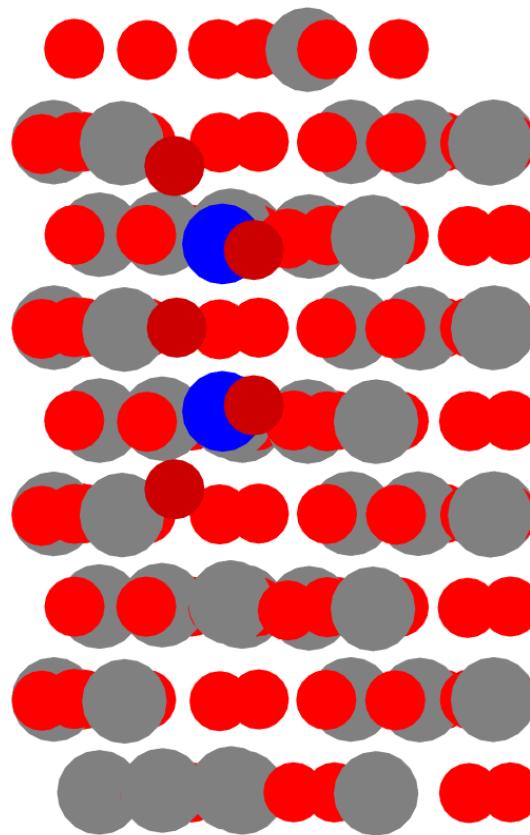
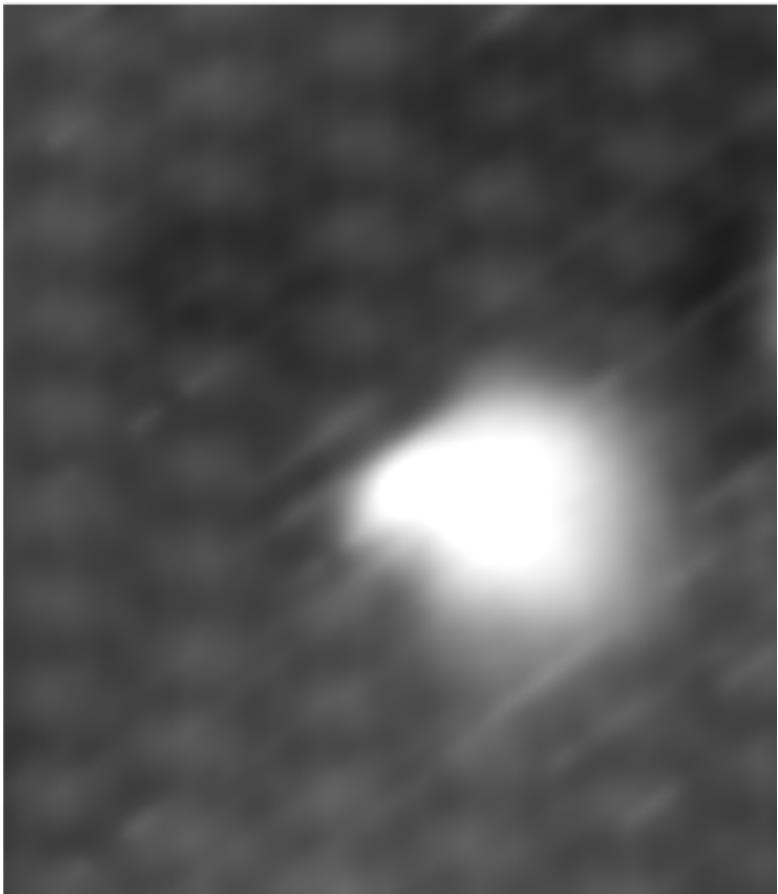
2xV  
6XO  
2XH

After Water Exposure



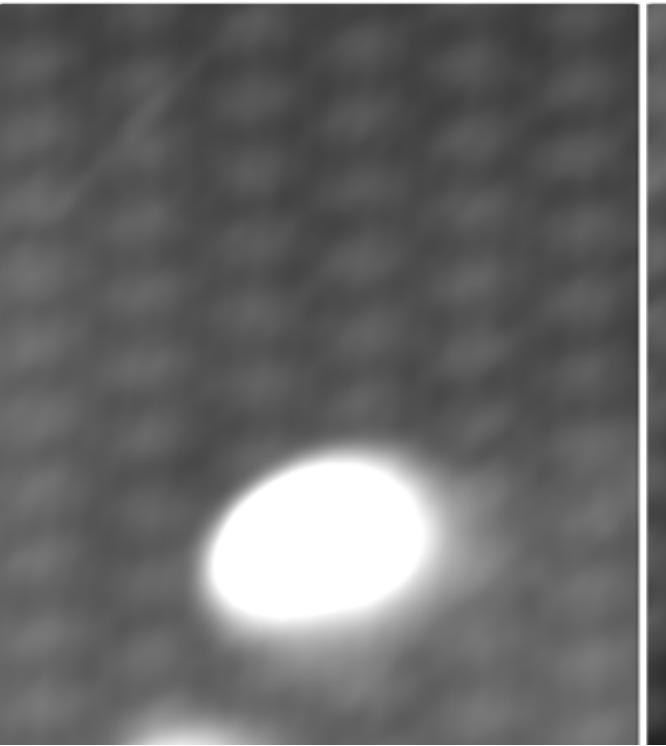
Placement of H is very  
uncertain

After Water Exposure

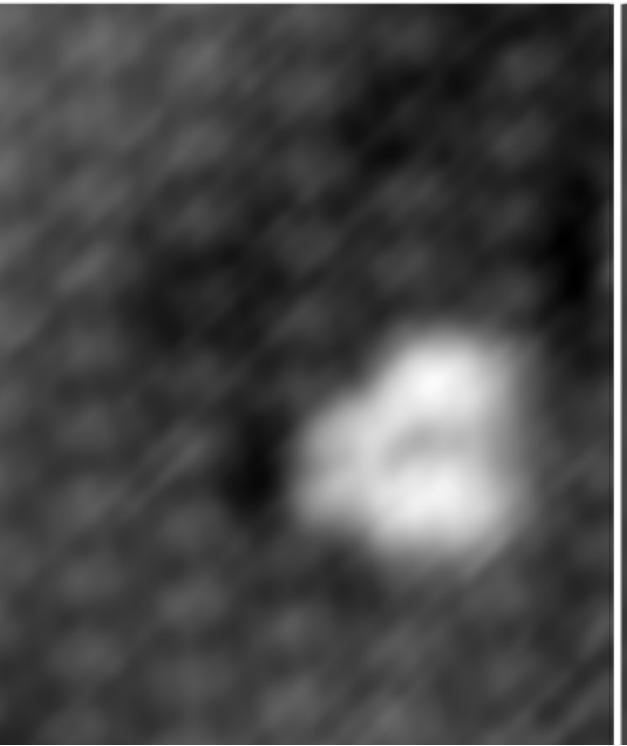


2xV  
5XO

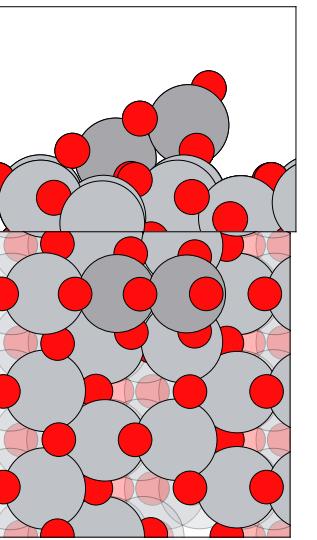
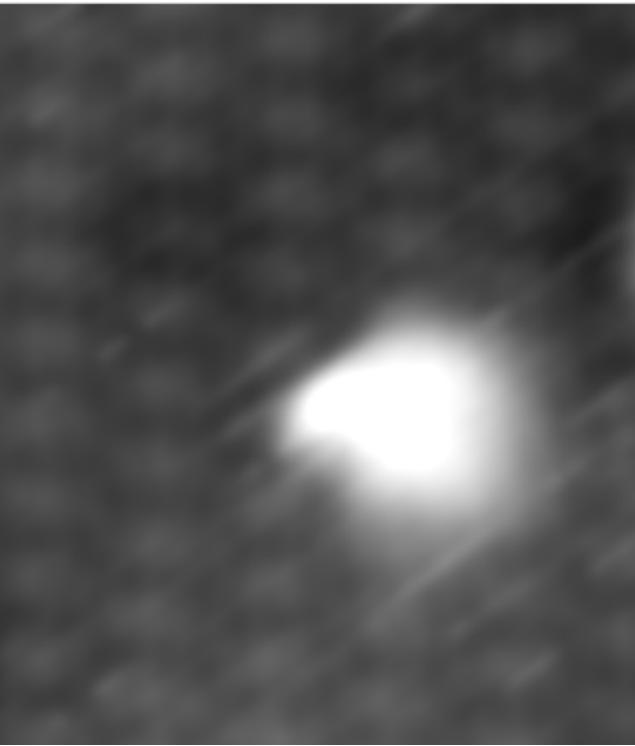
As-Deposited



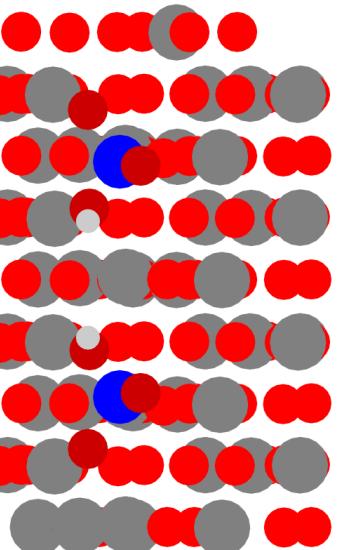
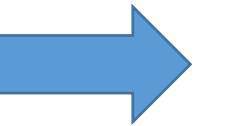
During Water exposure



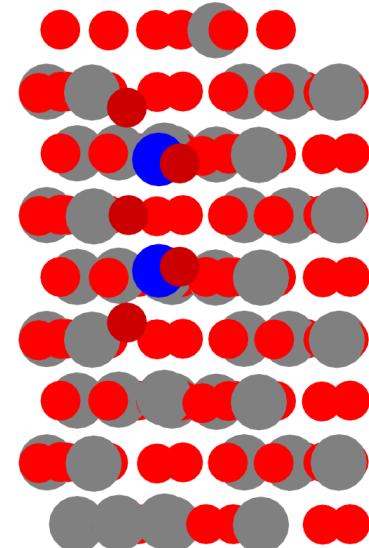
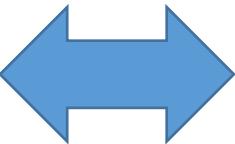
After Water Exposure



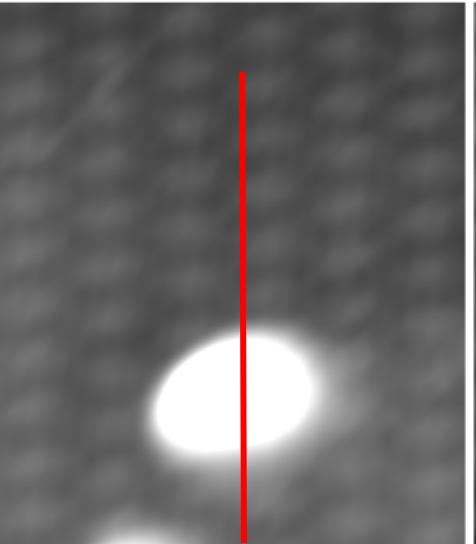
$1 \times H_2O$



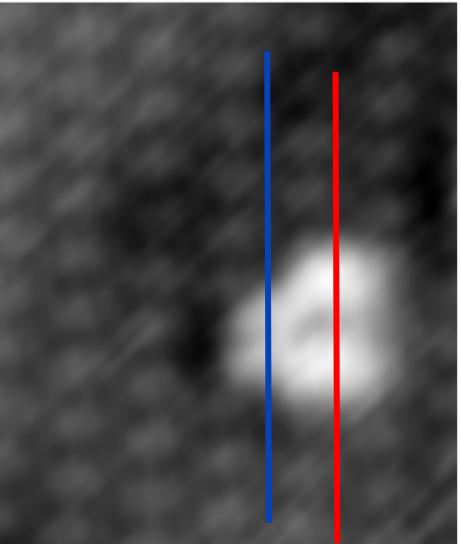
$H_2O$



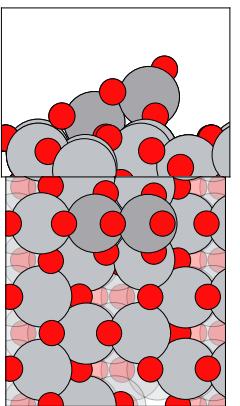
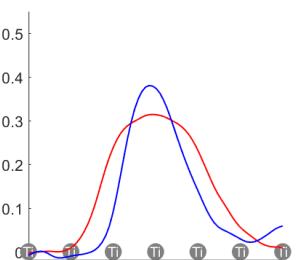
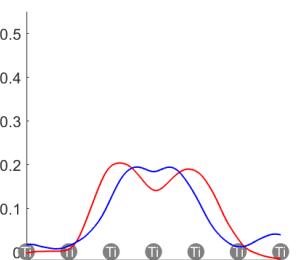
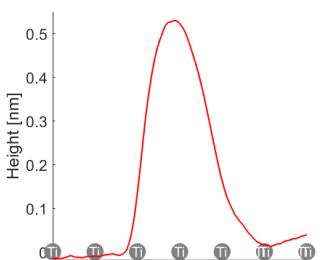
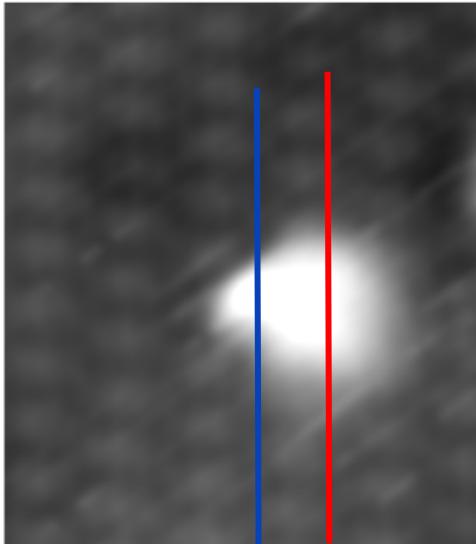
As-Deposited



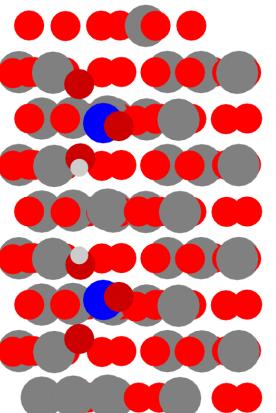
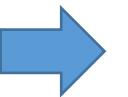
During Water exposure



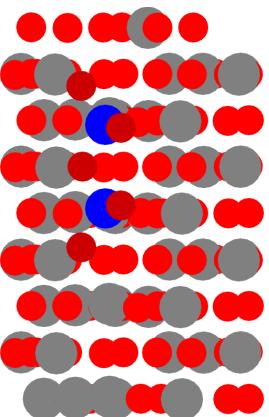
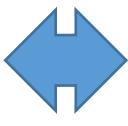
After Water Exposure



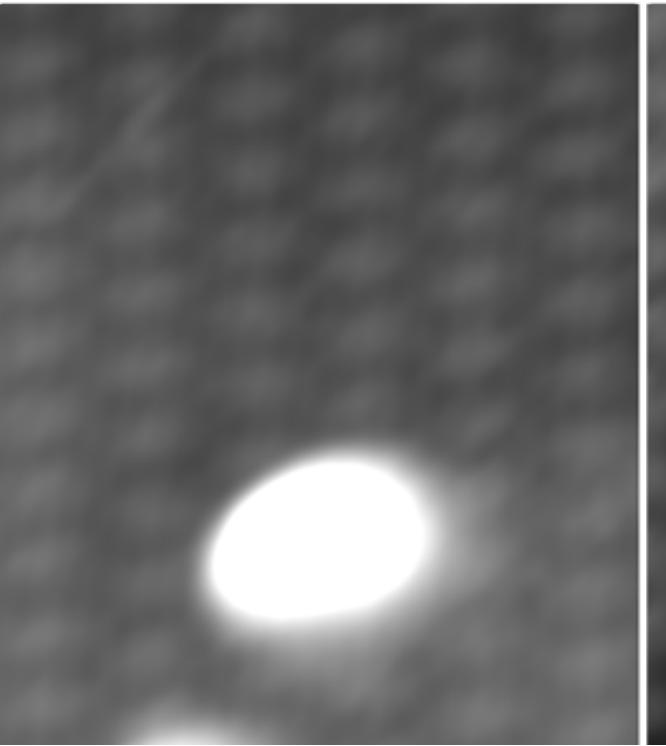
$1 \times H_2O$



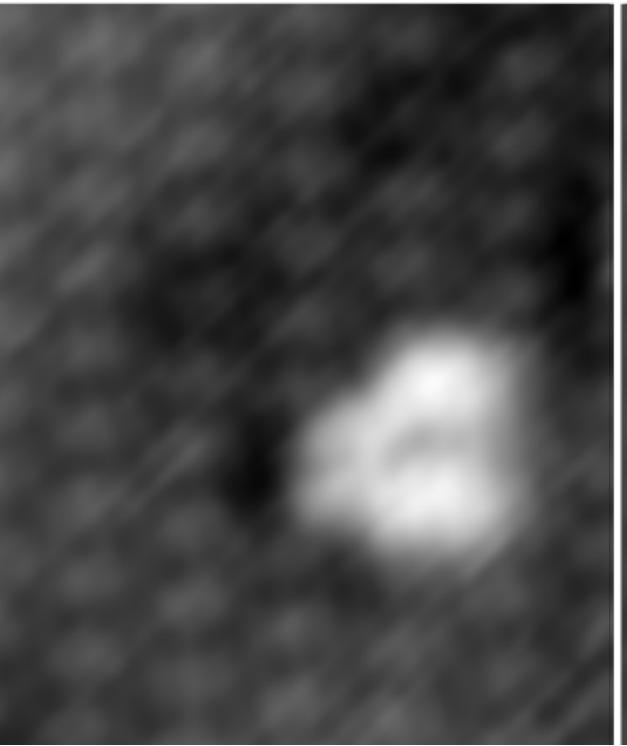
$H_2O$



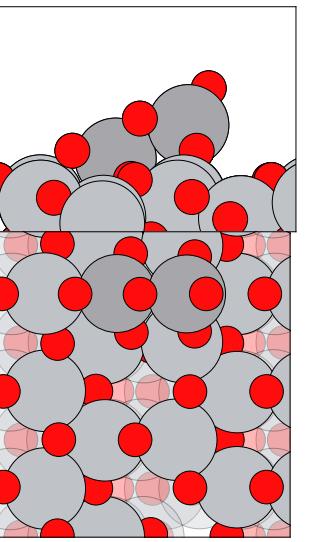
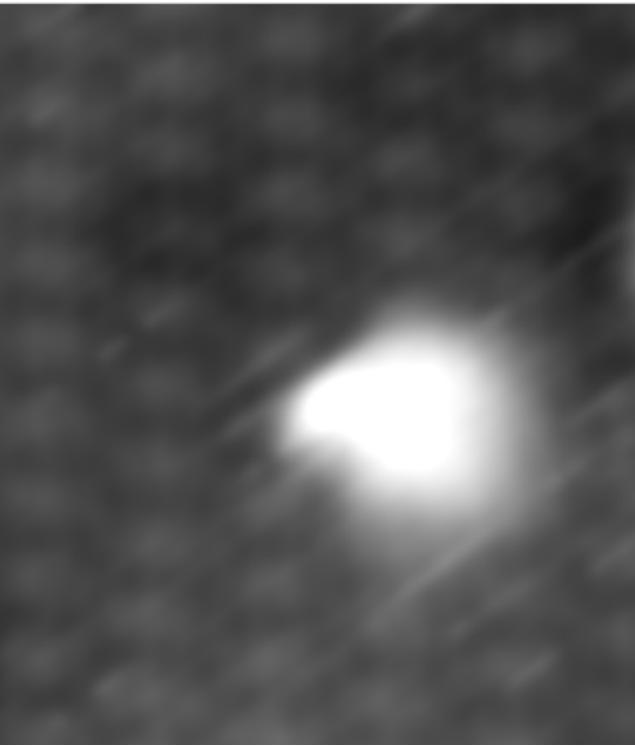
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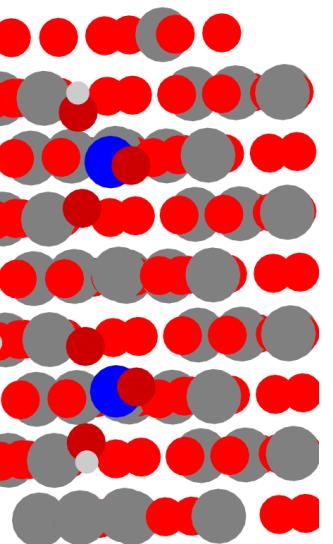
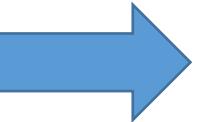
During Water exposure



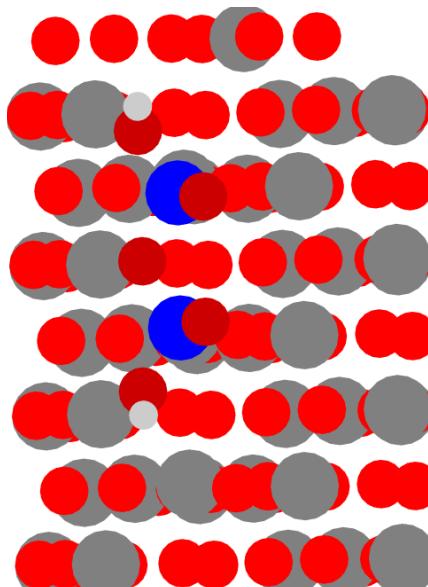
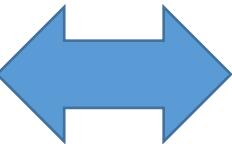
After Water Exposure



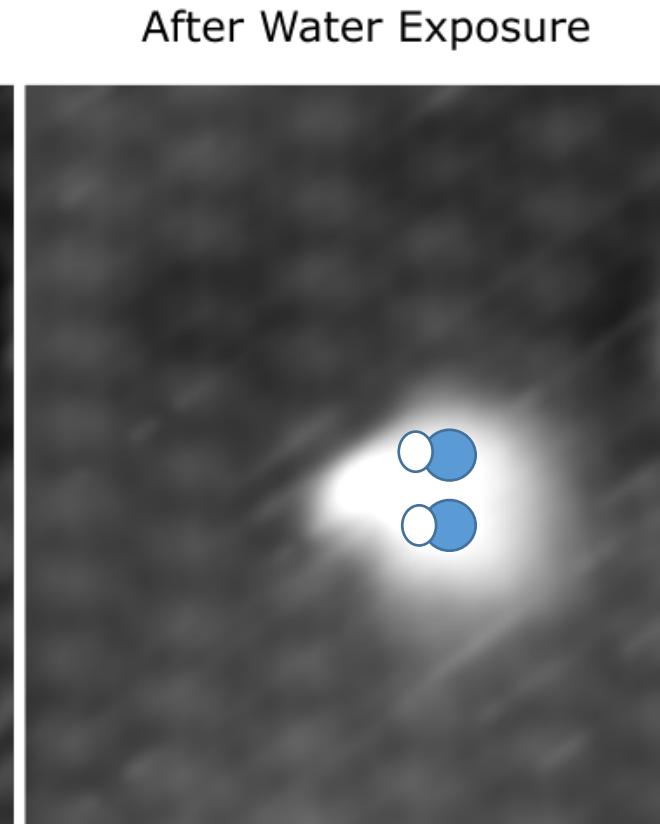
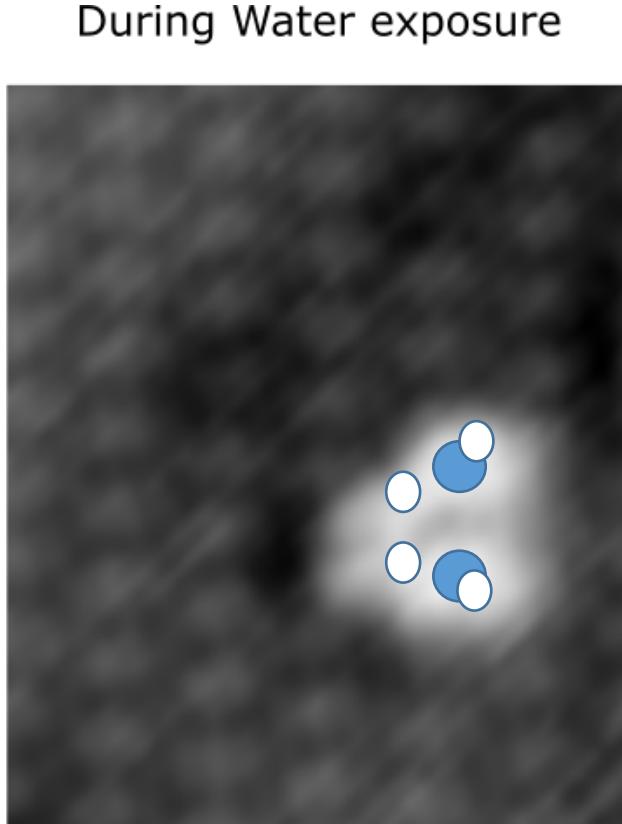
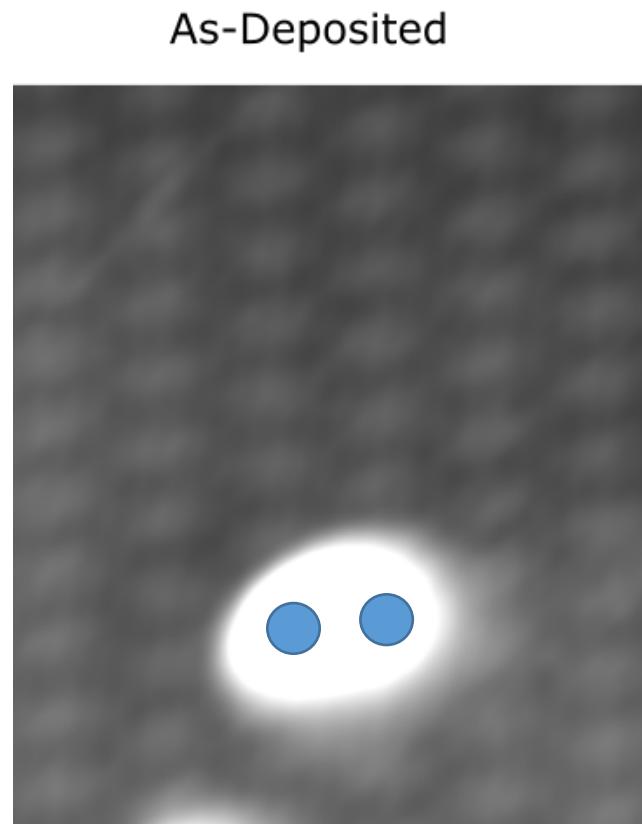
$1 \times H_2O$   
 $2 \times H$



$H_2O$



# model suggestions

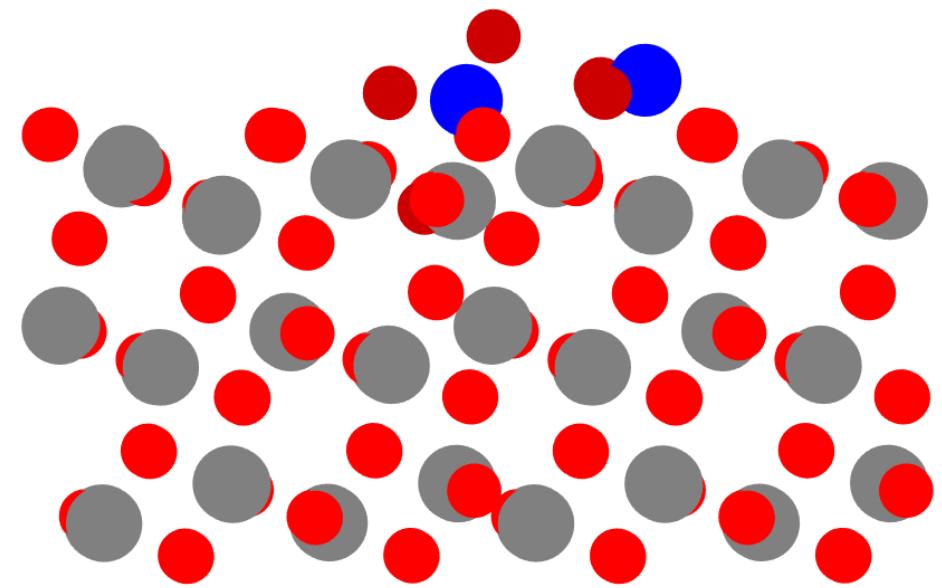
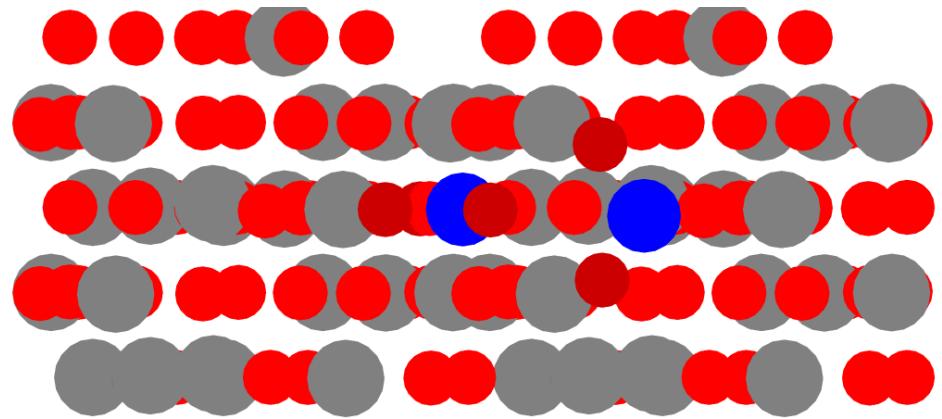
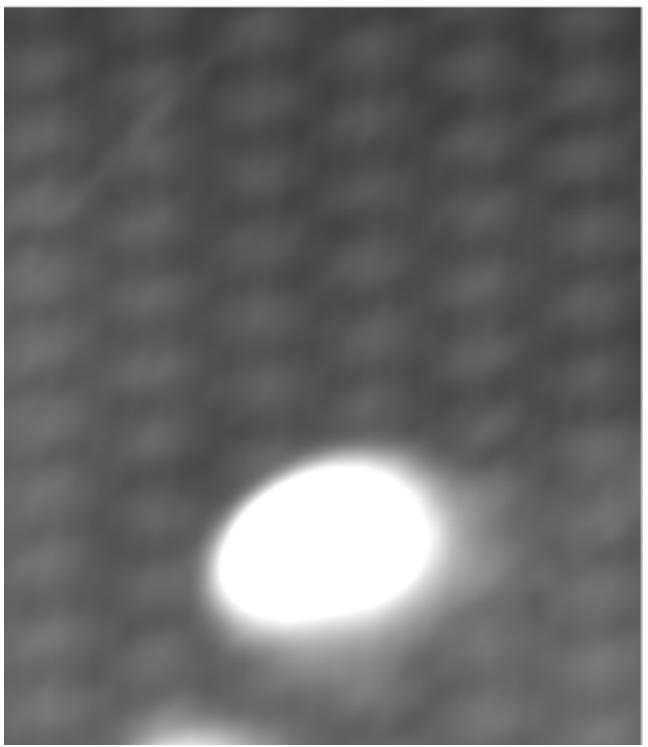


$2 \times \text{VO}_2$   
2 different configurations

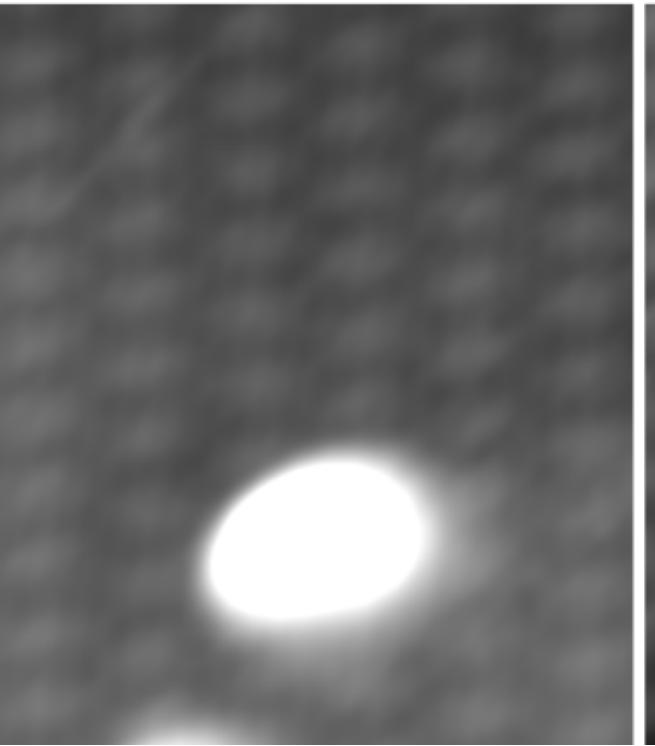
$2 \times \text{VO}_3\text{H} + 2 \times \text{H}_{\text{bridge}}$

$\text{V}_2\text{O}_5\text{H}_2$

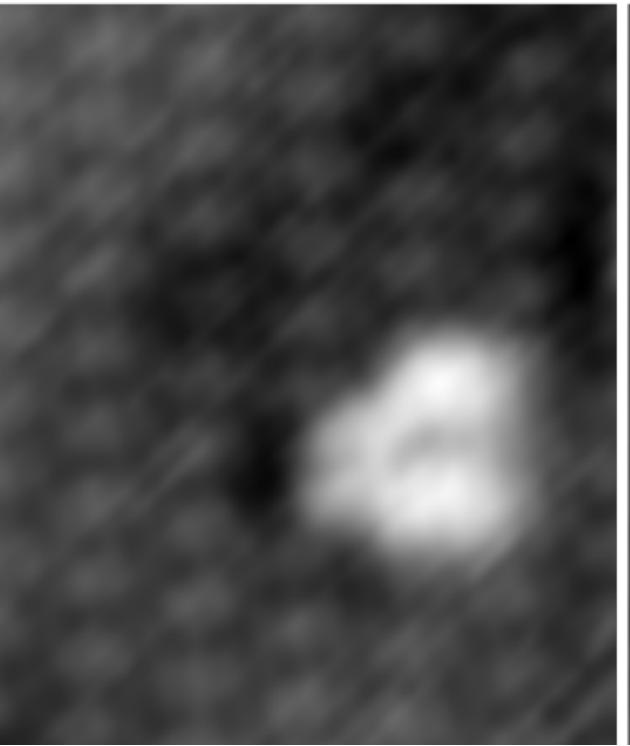
As-Deposited



As-Deposited



During Water exposure



After Water Exposure

