Water induced Restructuring of Vanadia clusters supported on a-TiO$_2$ (101) hydration dynamics

(Dated: 5 March 2020)
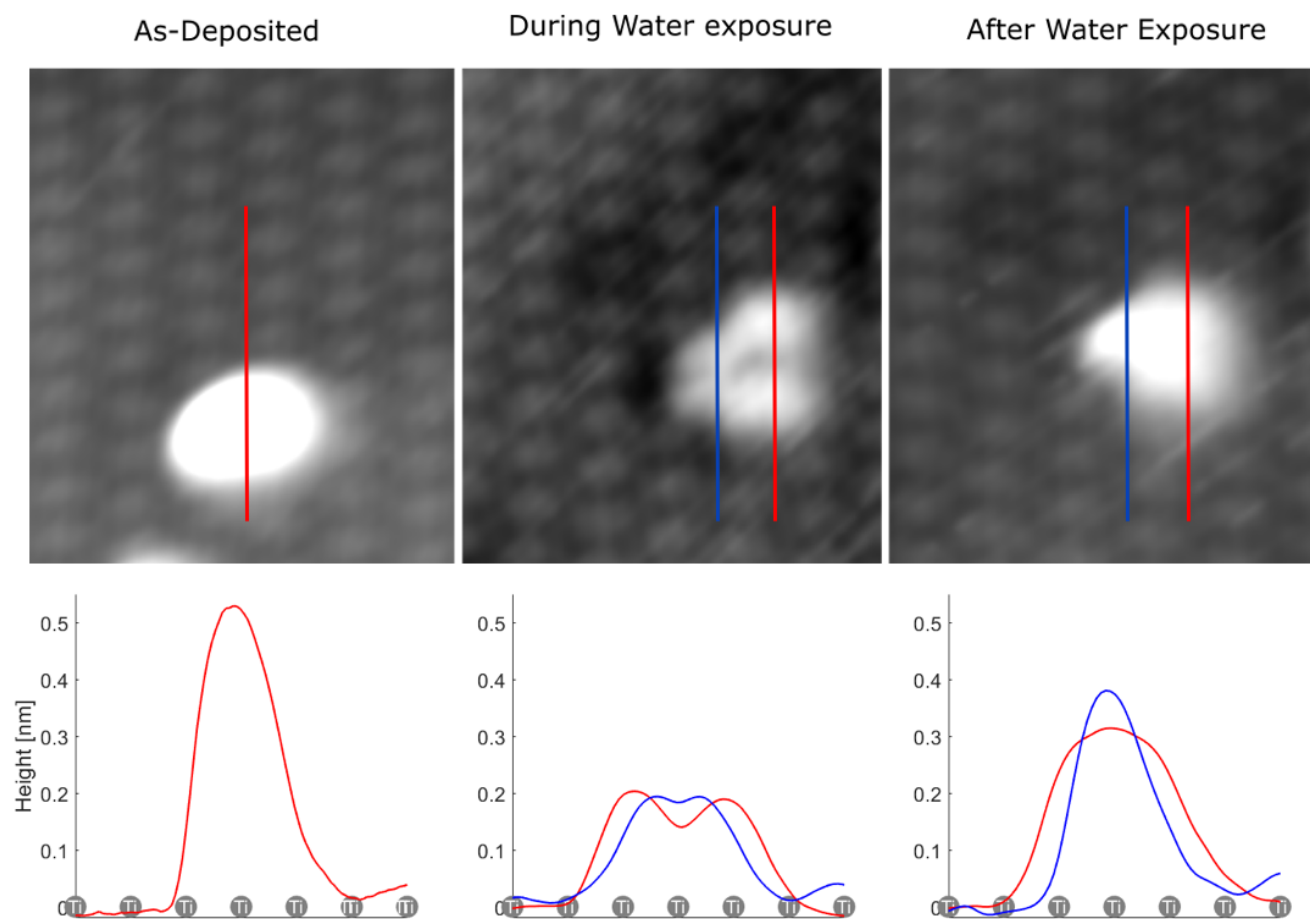
FIG. 1. Experimental Observation
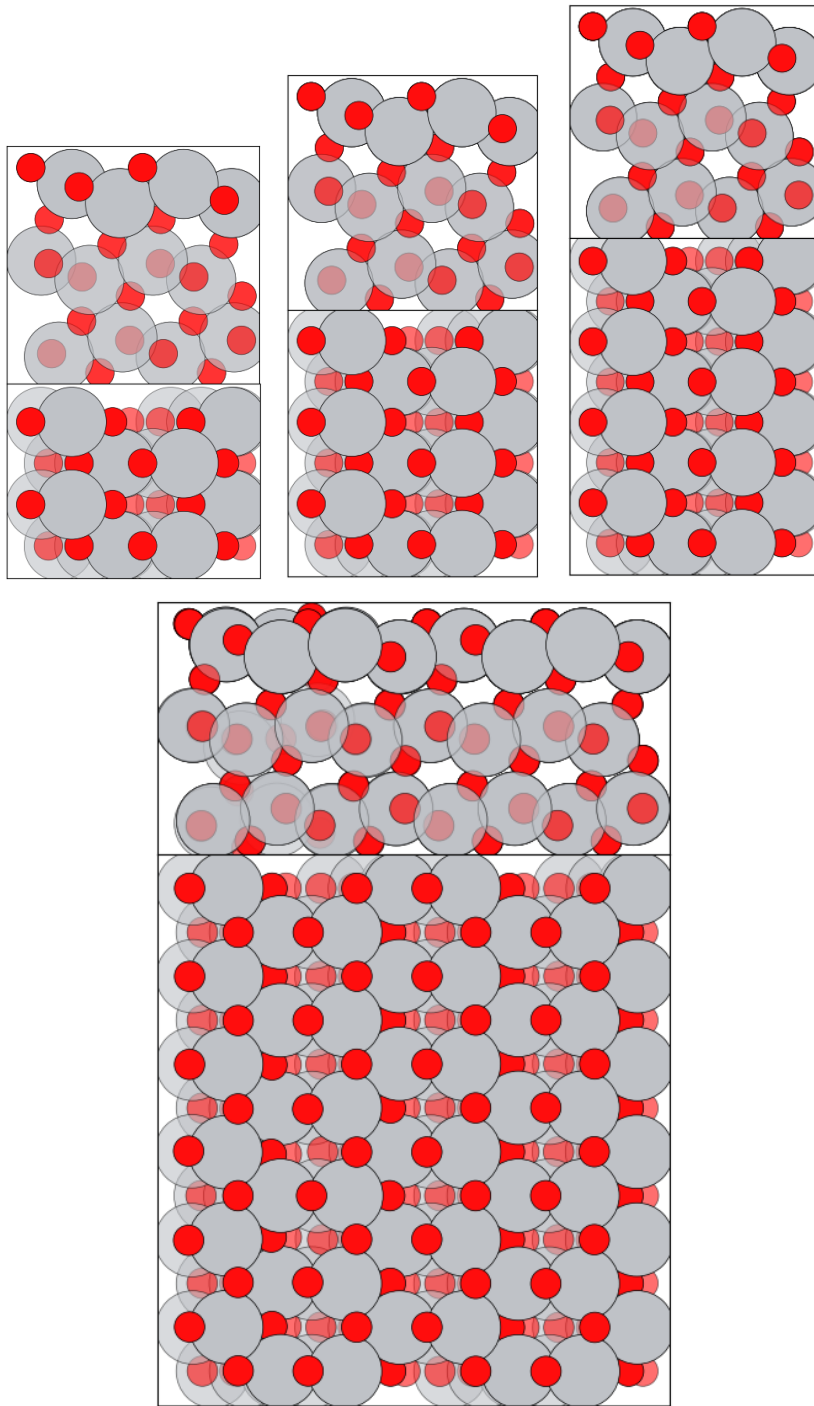
FIG. 2. Different super cell size of surfaces used in all the calculations.

I1: $\Delta E = 0.000\ eV$ I1: $\Delta E = 0.000\ eV$ I2: $\Delta E = 0.131\ eV$ I3: $\Delta E = 0.162\ eV$ I4: $\Delta E = 0.230\ eV$

I1: $\Delta E = 0.000\ eV$ I2: $\Delta E = 0.021\ eV$ I3: $\Delta E = 0.053\ eV$ I4: $\Delta E = 0.071\ eV$ I5: $\Delta E = 0.176\ eV$ I6: $\Delta E = 0.208\ eV$
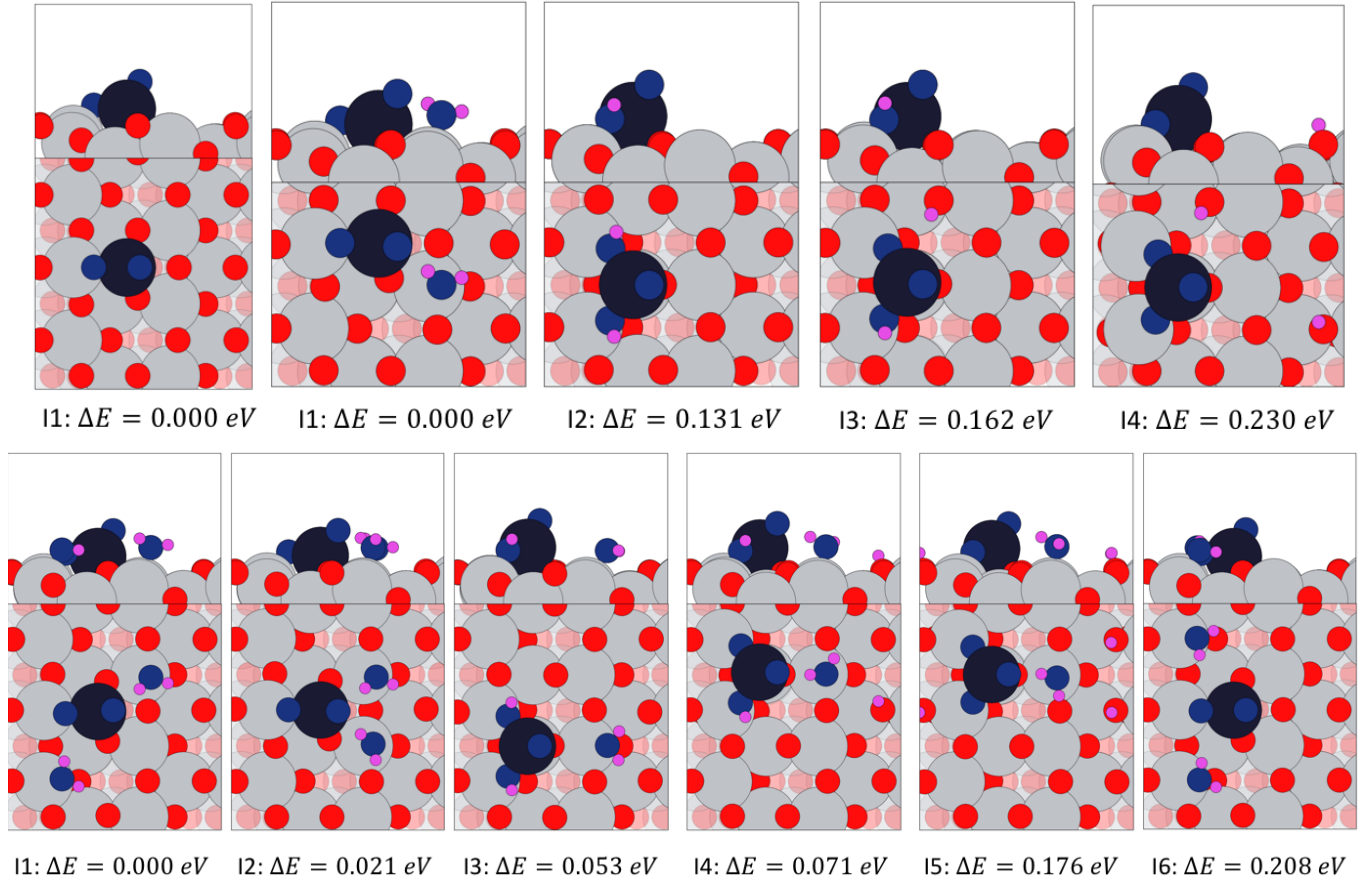
FIG. 3. All the possible low-lying isomers found for VO_2 , VO_2H_2O and $VO_2 2H_2O$ clusters with GOFEE were DFT relaxed with one Oxygen vacancy created in 2nd layer. Here two types of super cell sizes were used those are $2 \times 1 \times 1$ super cell for VO_2 , VO_2H_2O and $3 \times 1 \times 1$ super cell for $VO_2 2H_2O$ clusters.
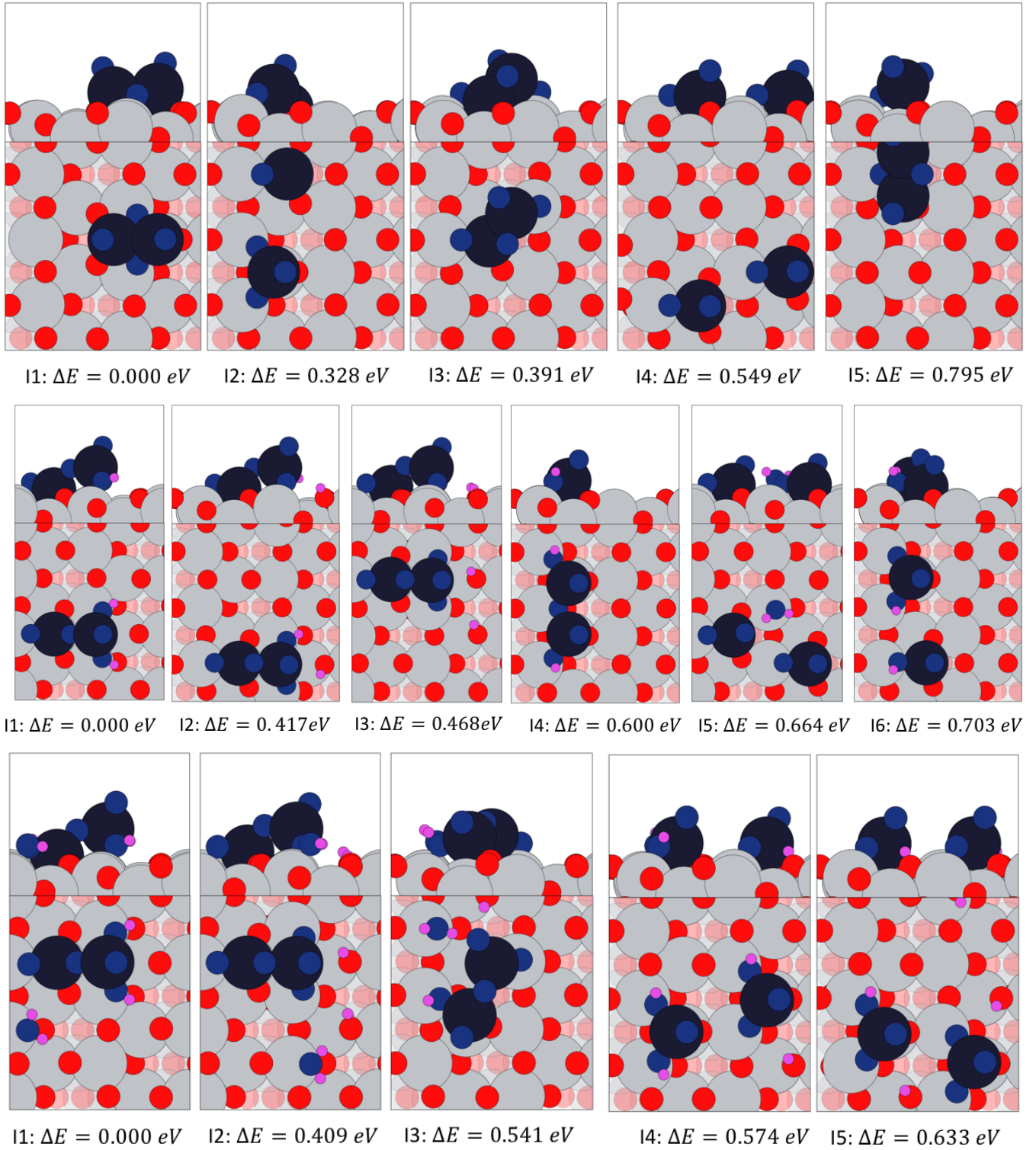
FIG. 4. All the possible low-lying isomers found for V_2O_4 , V_2O_4 H_2O and V_2O_4 $2H_2O$ clusters with GOFEE were DFT relaxed with one Oxygen vacancy created in 2nd layer. Here $3 \times 1 \times 1$ super cell used for all clusters.

FIG. 5. All the possible low-lying isomers found for V_2O_5 , $V_2O_5H_2O$ and $V_2O_52H_2O$ clusters with GOFEE were DFT relaxed with one Oxygen vacancy created in 2nd layer. Here $4 \times 1 \times 1$ super cell used for all clusters.
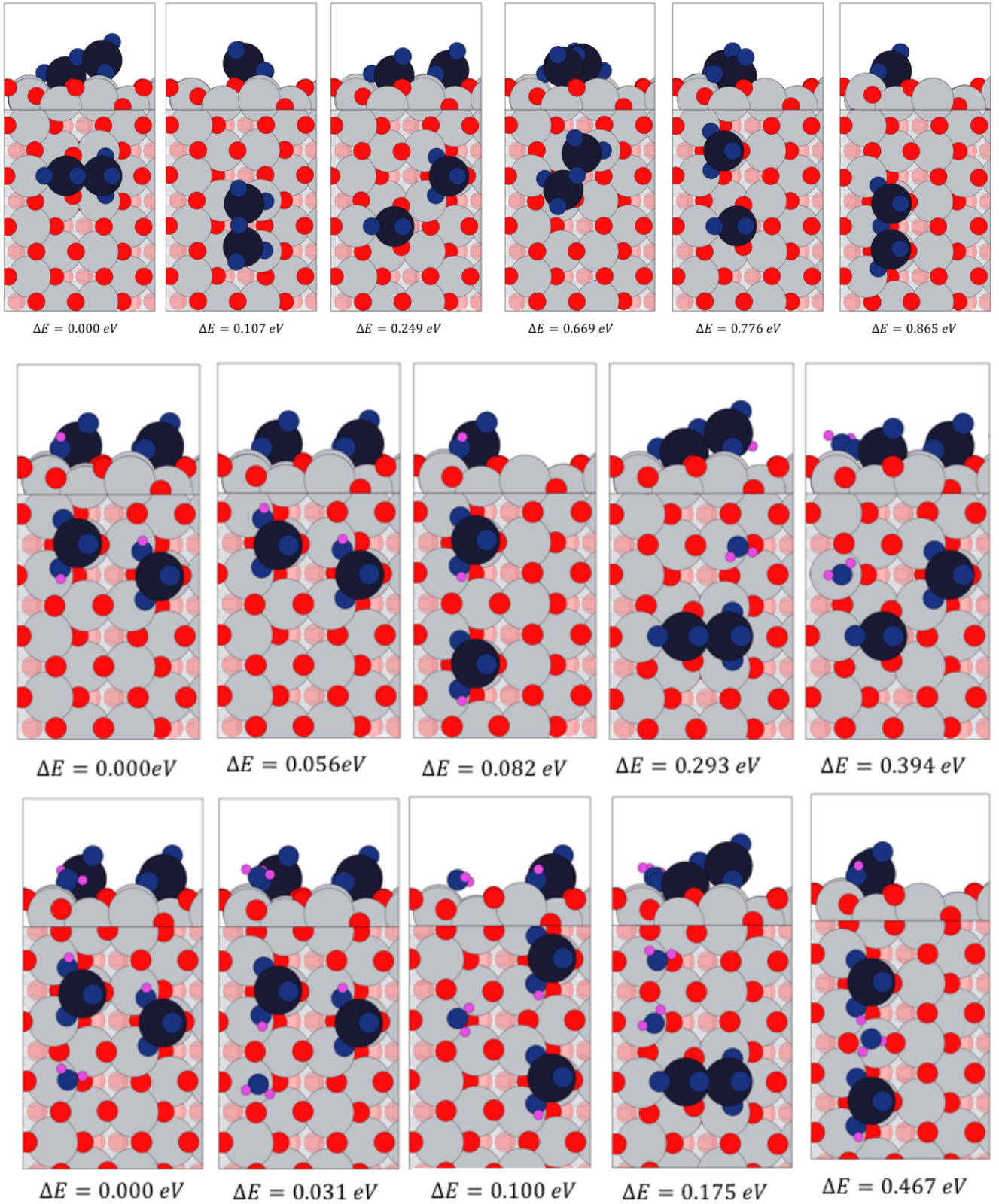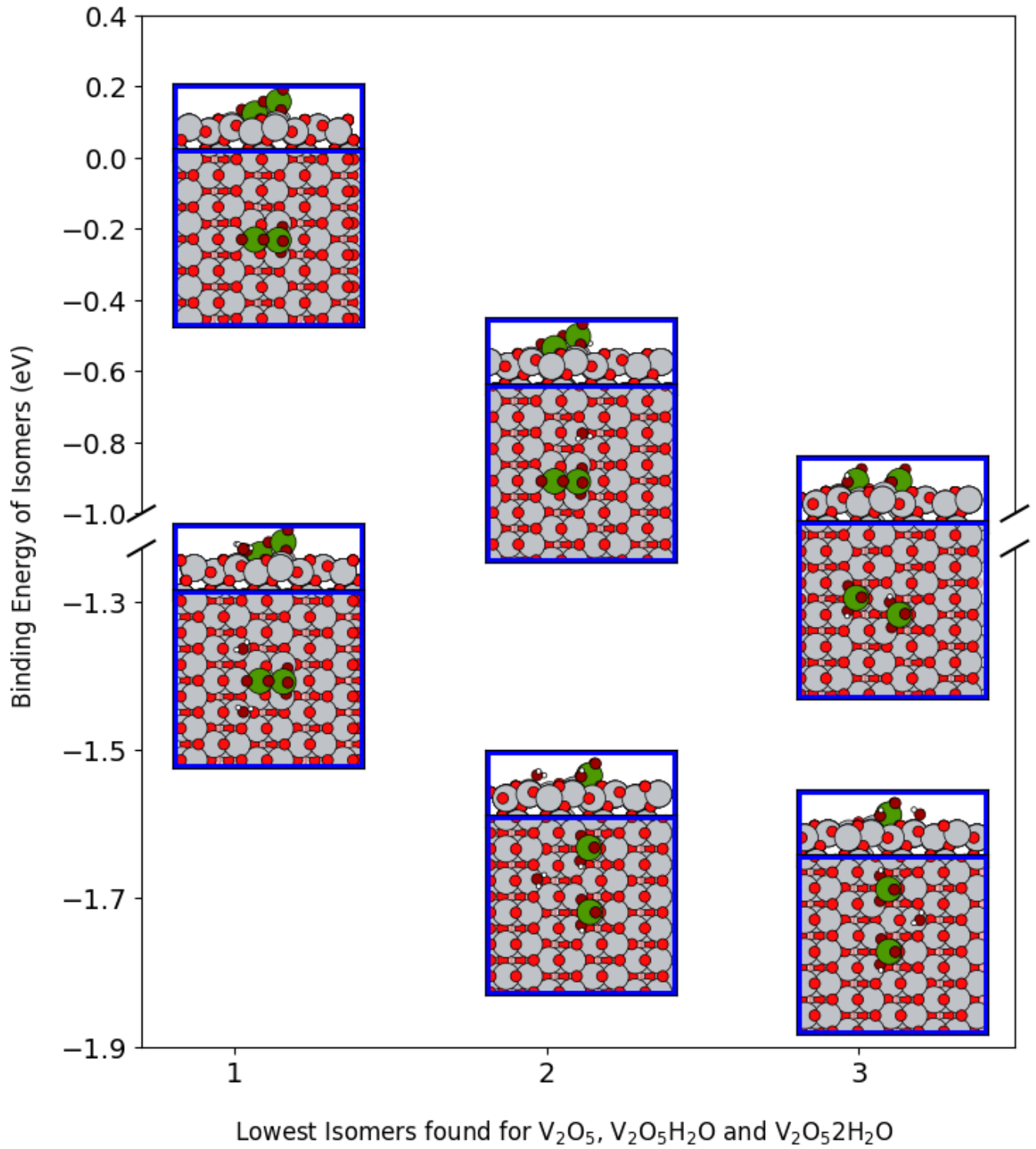
FIG. 6. Binding energy order for best structures of V_2O_5 , V_2O_5 H_2O and V_2O_5 $2H_2O$ clusters found in global optimization were re-optimised with $6 \times 2 \times 1$ super cell and one oxygen vacancy created.

FIG. 7. Binding energy order for best structures of V_2O_5, V_2O_5 H_2O and V_2O_5 $2H_2O$ clusters found in global optimization were re-optimised with $6 \times 2 \times 1$ s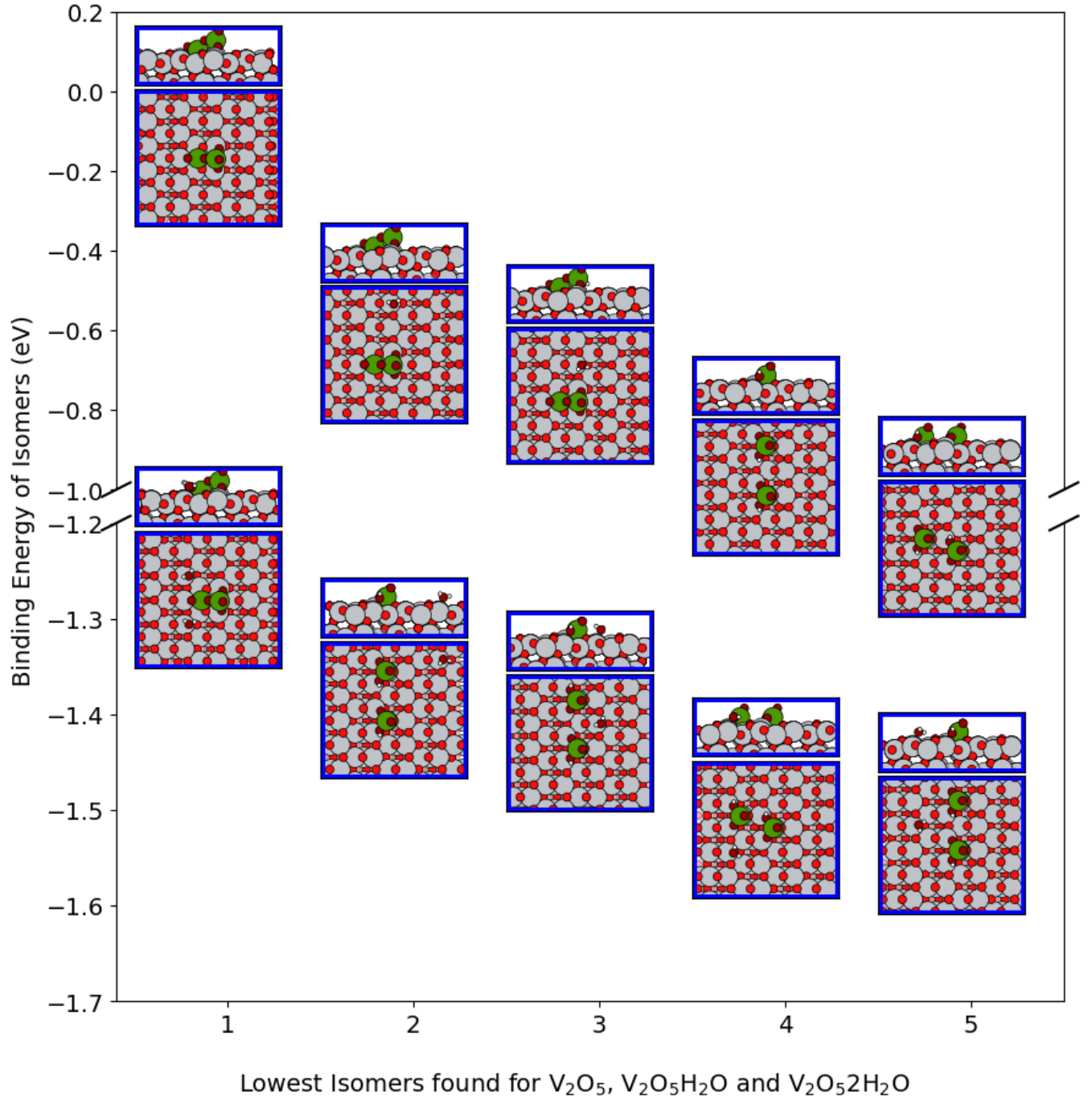uper cell and two oxygen vacancy created.