Water induced Restructuring of Vanadia clusters supported on a-TiO_2 (101) hydration dynamics

(Dated: 5 March 2020)

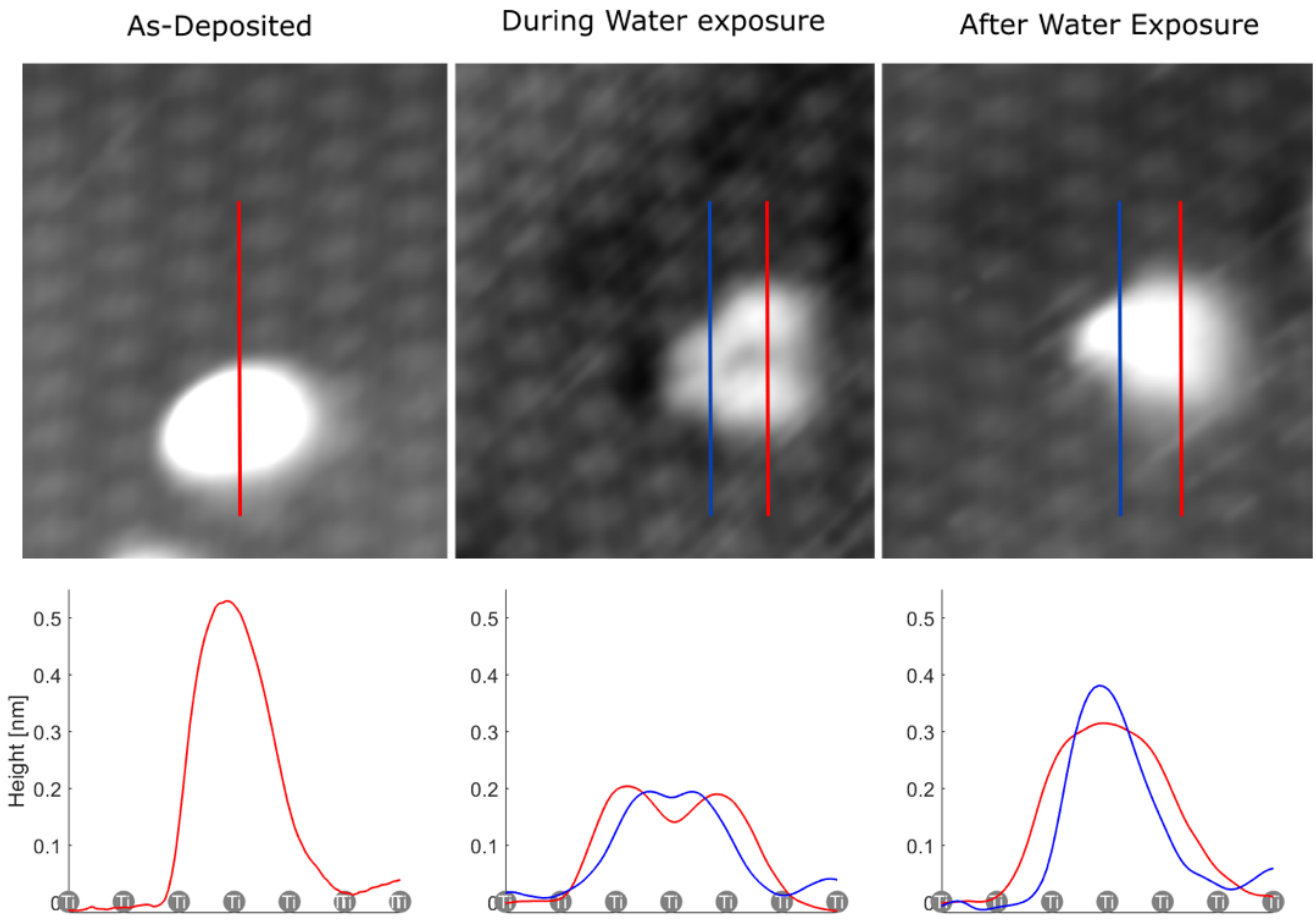

FIG. 1. Experimental Observation

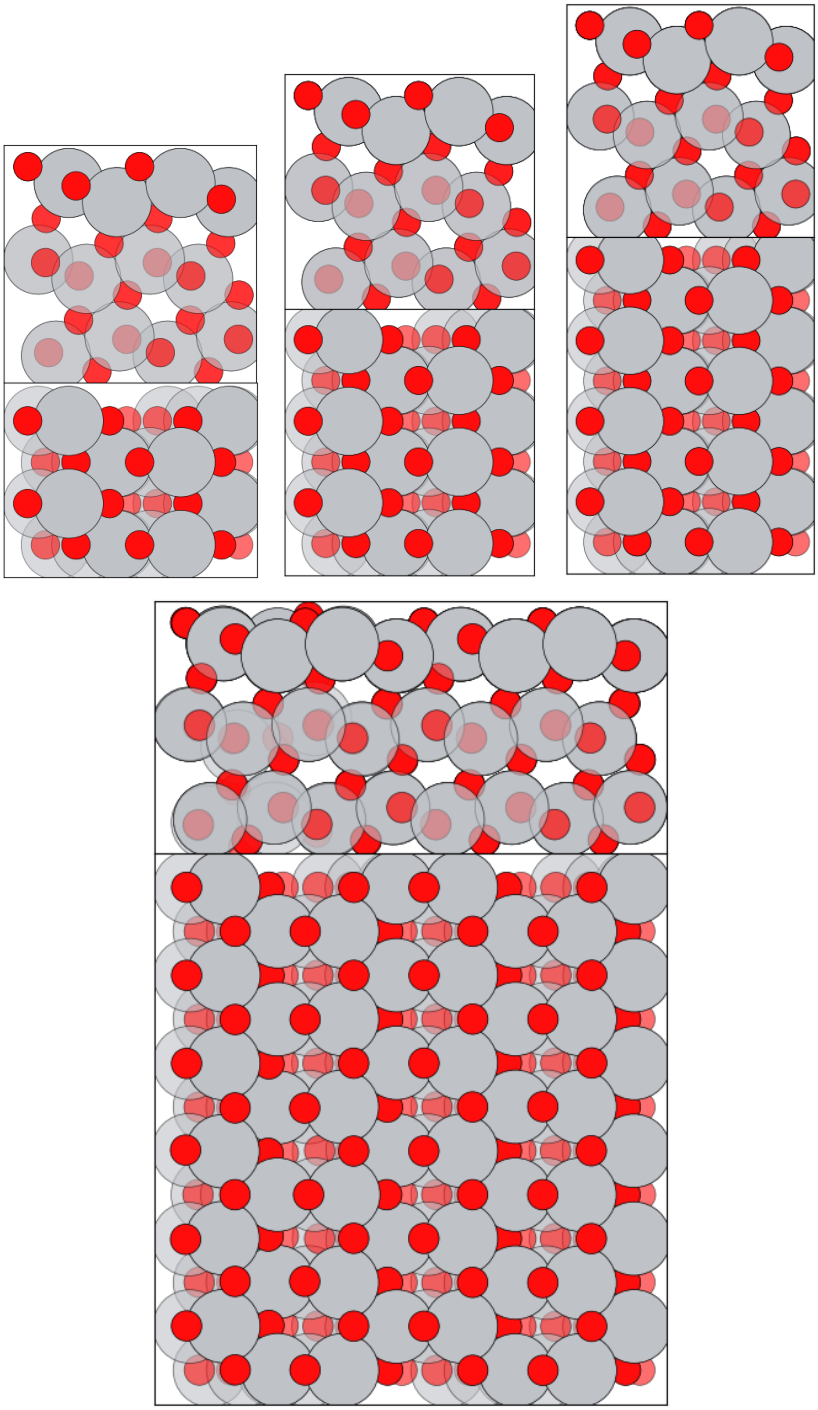

FIG. 2. Different super cell size of surfaces used in all the calculations.

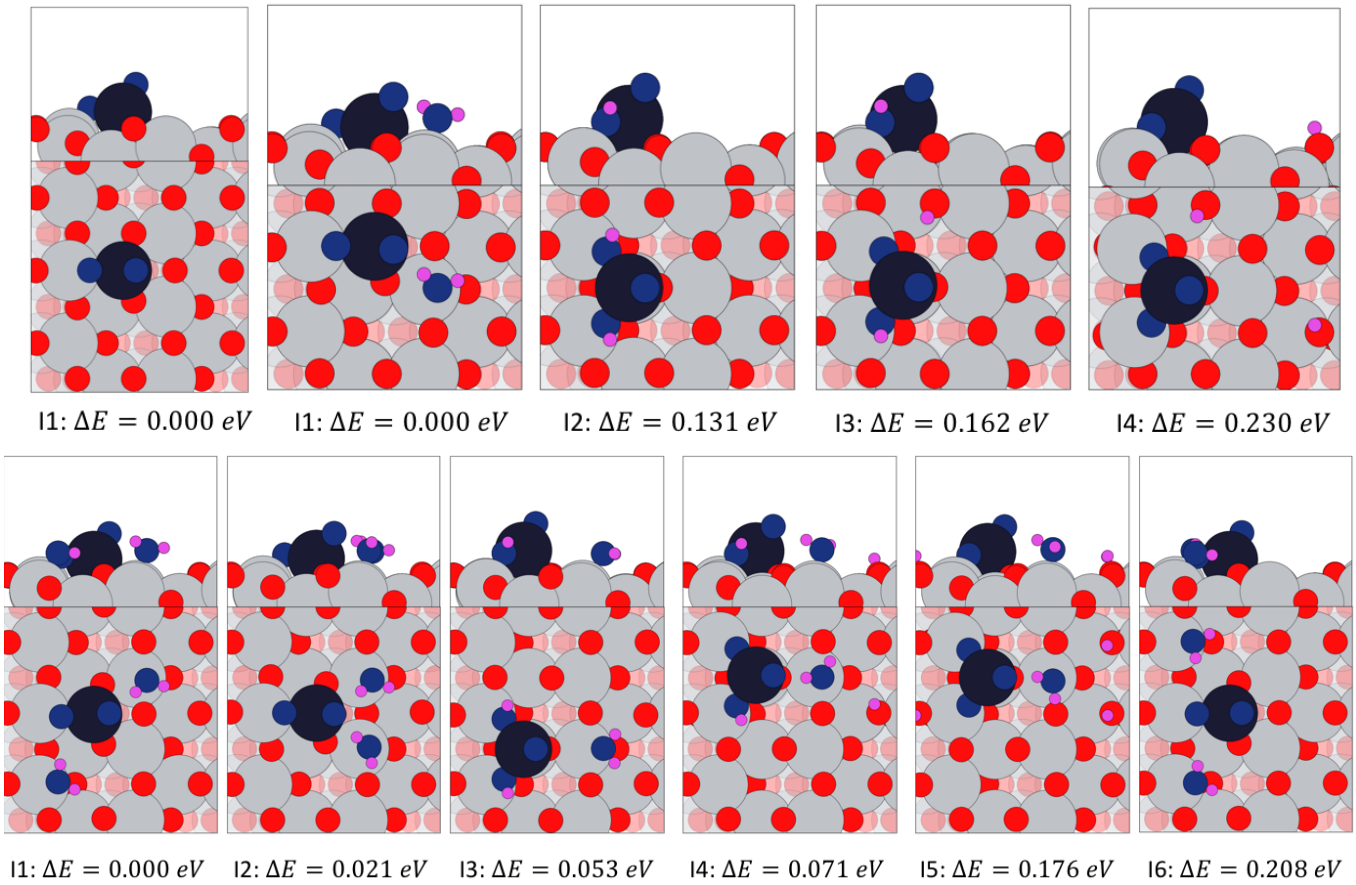

FIG. 3. All the possible low-lying isomers found for VO_2 , VO_2H_2O and $VO_2 2H_2O$ clusters with GOFEE were DFT relaxed with one Oxygen vacancy created in 2nd layer. Here two types of super cell sizes were used those are $2 \times 1 \times 1$ super cell for VO_2 , VO_2H_2O and $3 \times 1 \times 1$ super cell for $VO_2 2H_2O$ clusters.

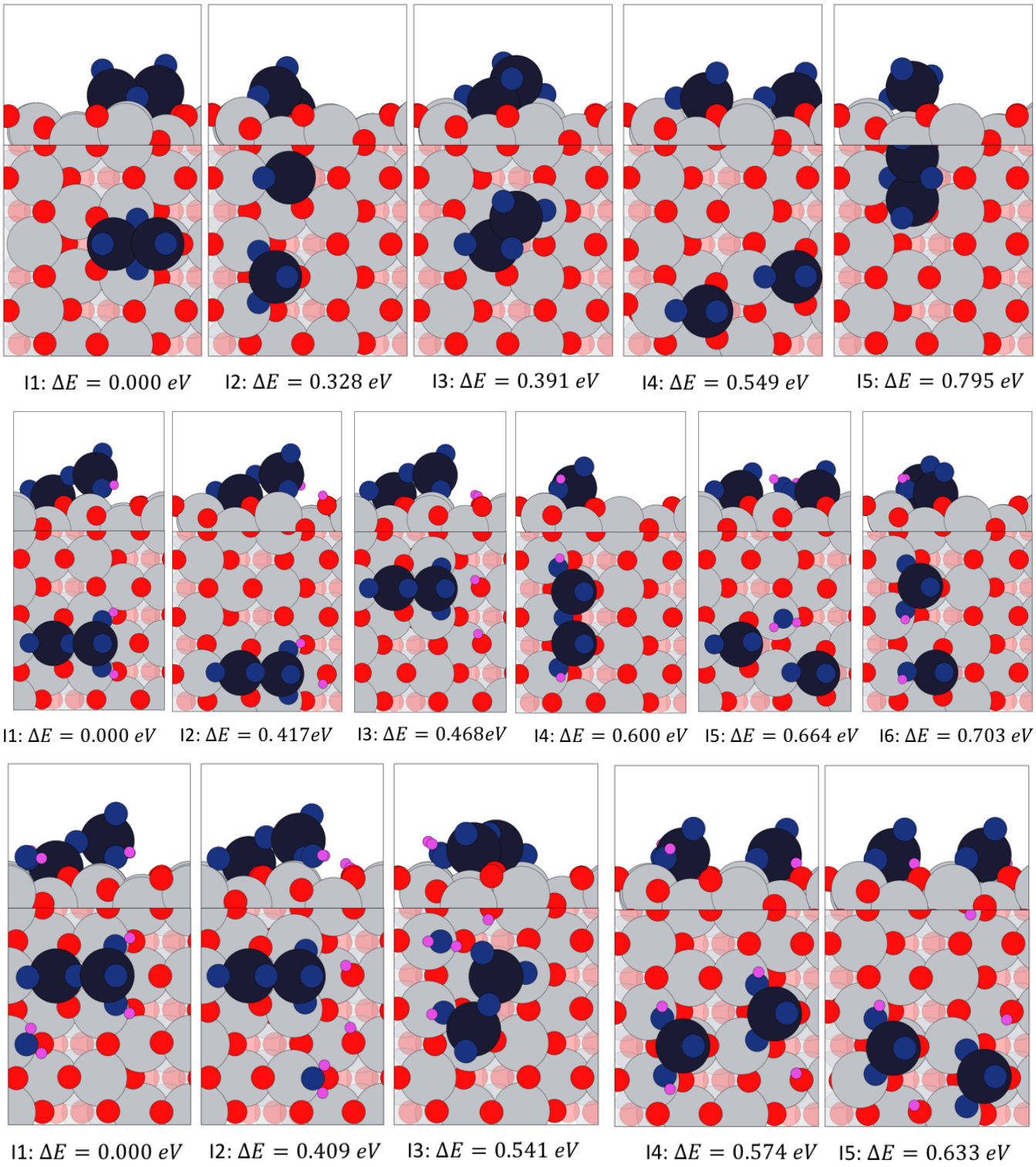

FIG. 4. All the possible low-lying isomers found for V_2O_4 , V_2O_4 H_2O and V_2O_4 $2H_2O$ clusters with GOFEE were DFT relaxed with one Oxygen vacancy created in 2nd layer. Here $3 \times 1 \times 1$ super cell used for all clusters.

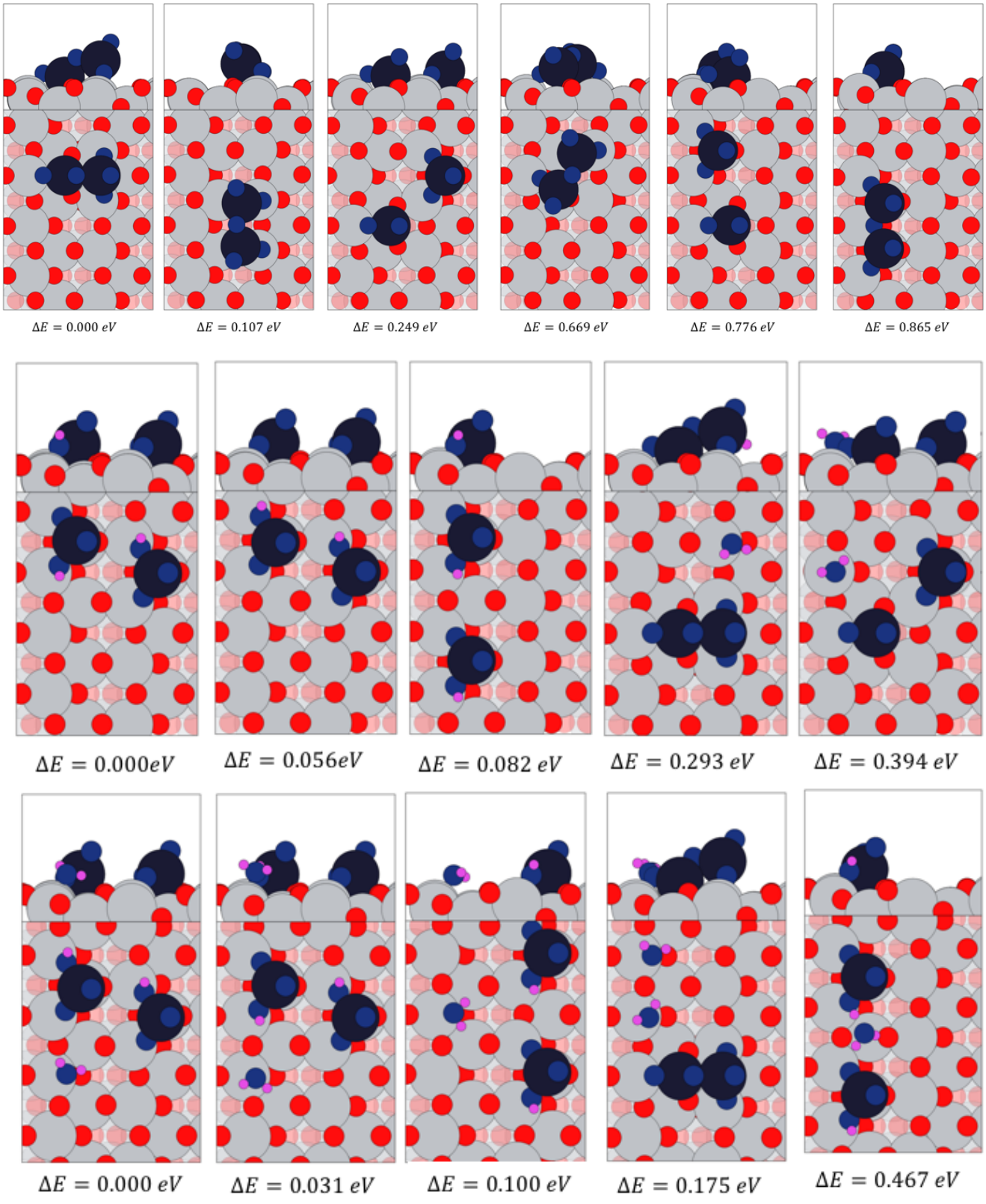

FIG. 5. All the possible low-lying isomers found for V_2O_5 , $V_2O_5H_2O$ and $V_2O_52H_2O$ clusters with GOFEE were DFT relaxed with one Oxygen vacancy created in 2nd layer. Here $4 \times 1 \times 1$ super cell used for all clusters.

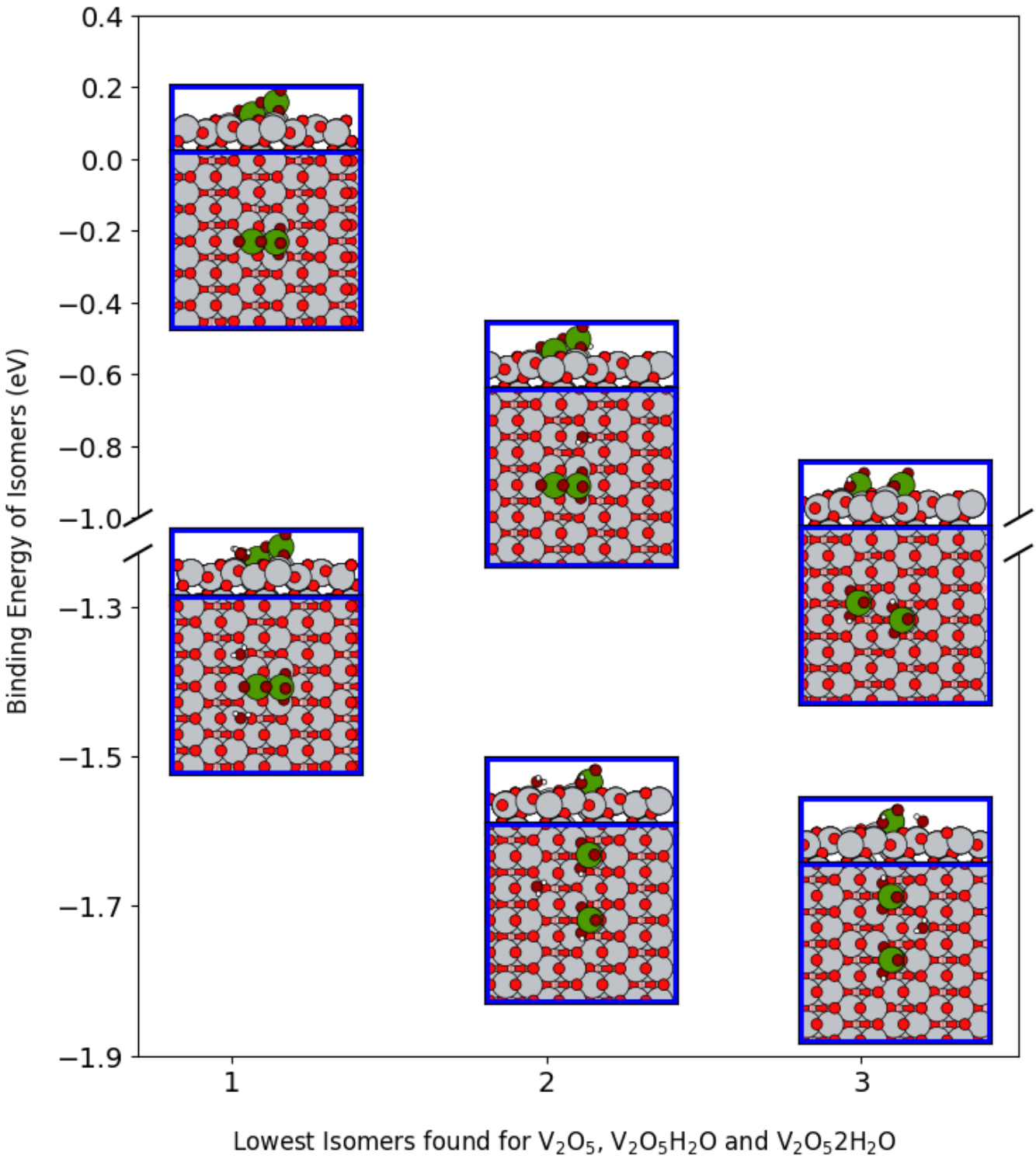

FIG. 6. Binding energy order for best structures of V_2O_5 , V_2O_5 H_2O and V_2O_5 $2H_2O$ clusters found in global optimization were re-optimised with $6 \times 2 \times 1$ super cell and one oxygen vacancy created.

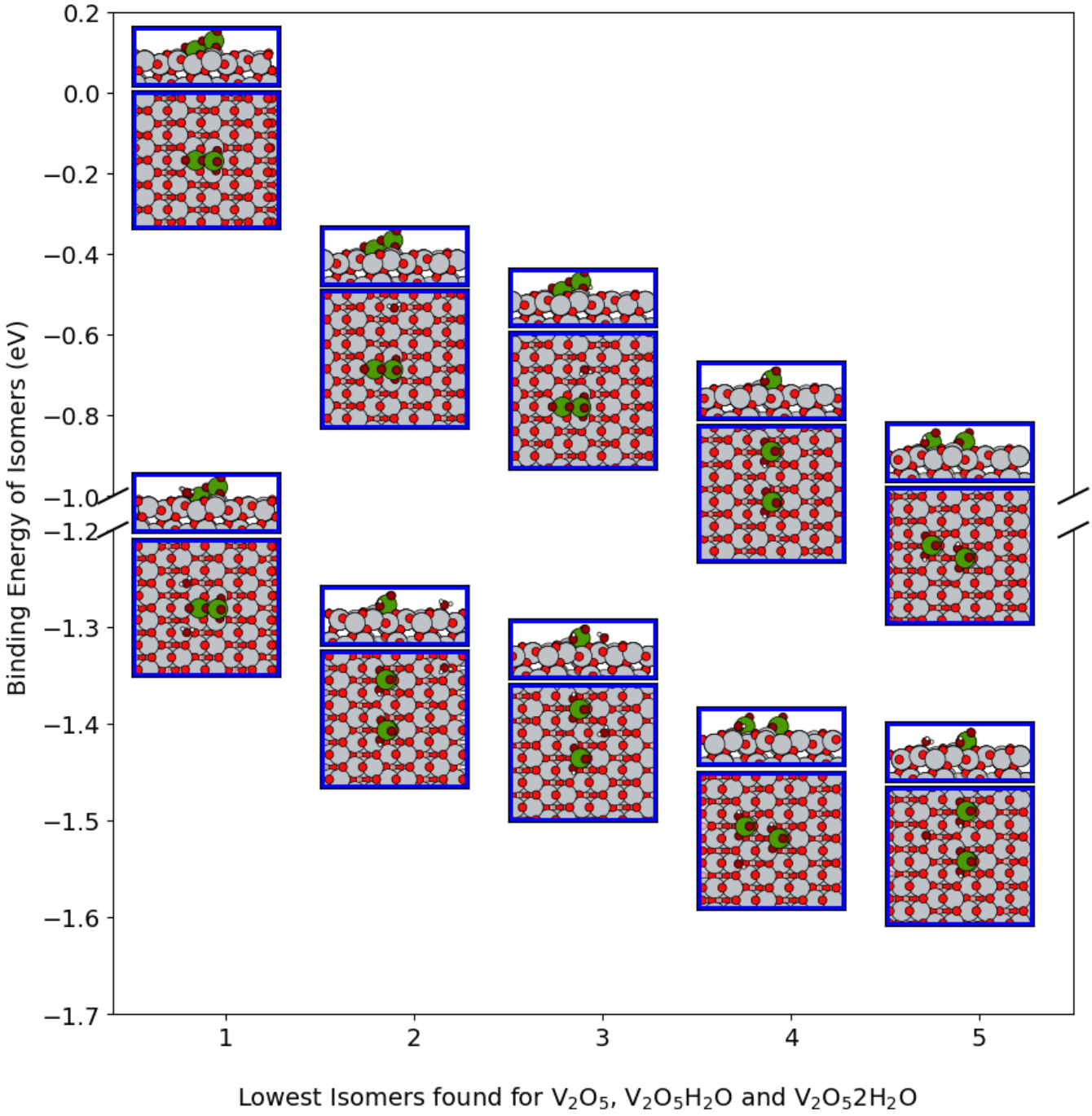

FIG. 7. Binding energy order for best structures of V_2O_5 , V_2O_5 H_2O and V_2O_5 $2H_2O$ clusters found in global optimization were re-optimised with $6 \times 2 \times 1$ super cell and two oxygen vacancy created.

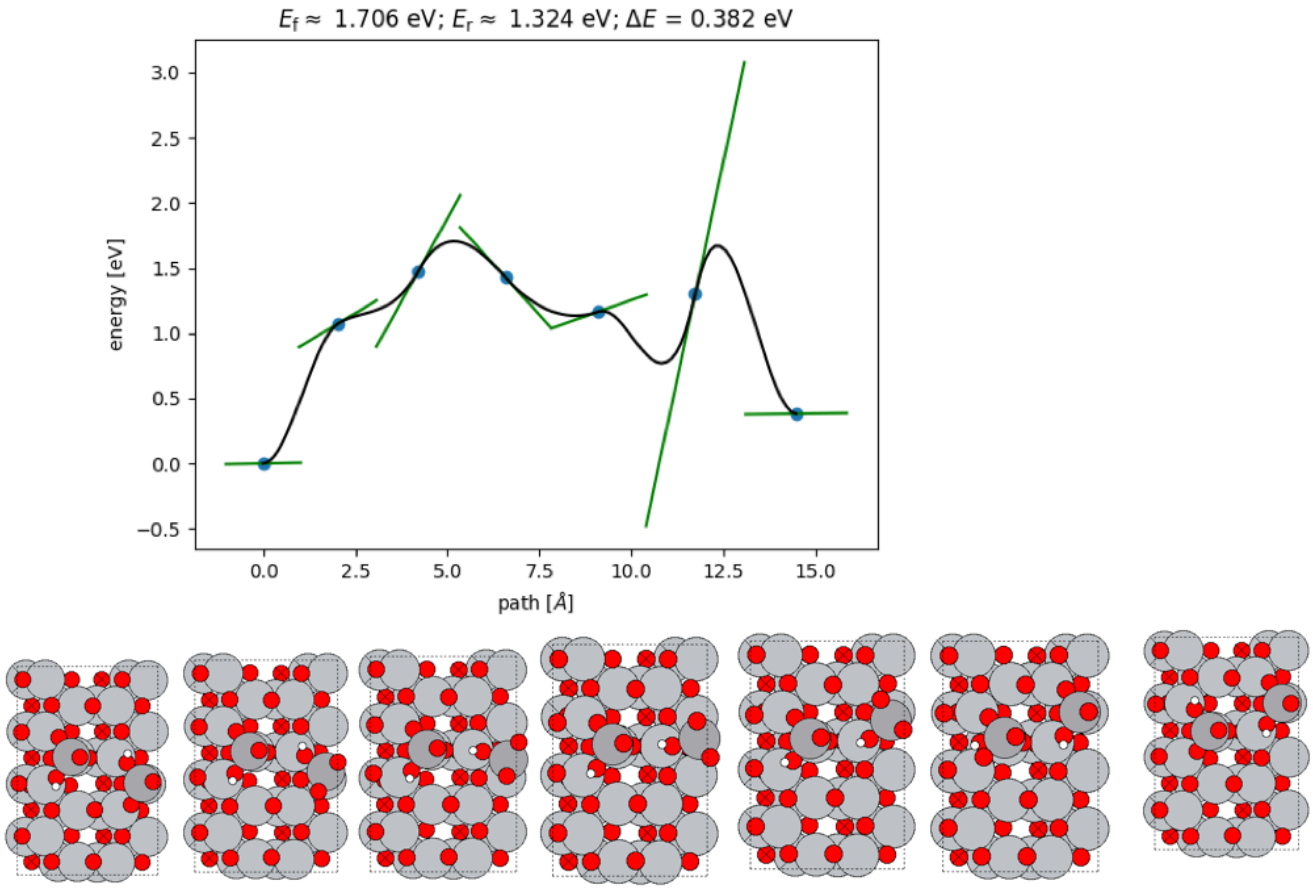

FIG. 8. NEB calculations