

Water induced Restructuring of Vanadia clusters supported on α -TiO₂ (101) hydration dynamics

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I. INTRODUCTION

II. EXPERIMENTAL CLAIM

III. METHODOLOGY

IV. RESULTS

A. low-lying isomers found for VO₂ , VO₂H₂O and VO₂2H₂O clusters

B. low-lying isomers found for V₂O₄ , V₂O₄H₂O and V₂O₄2H₂O clusters

C. low-lying isomers found for V₂O₅ , V₂O₅H₂O and V₂O₅2H₂O clusters

D. Binding Energies for V₂O₅ , V₂O₅H₂O and V₂O₅2H₂O clusters

V. REFERENCES

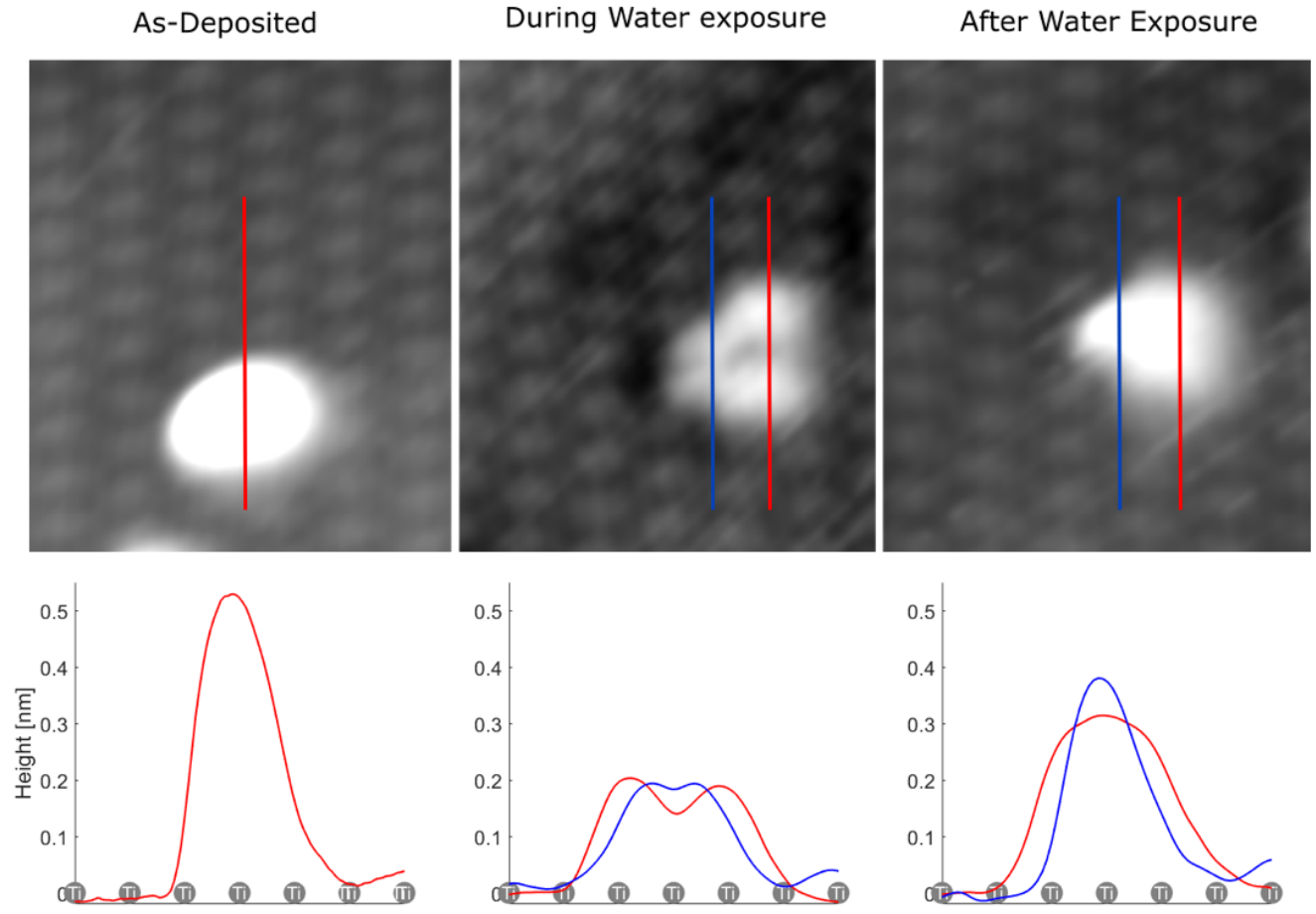


FIG. 1. Experimental Observation

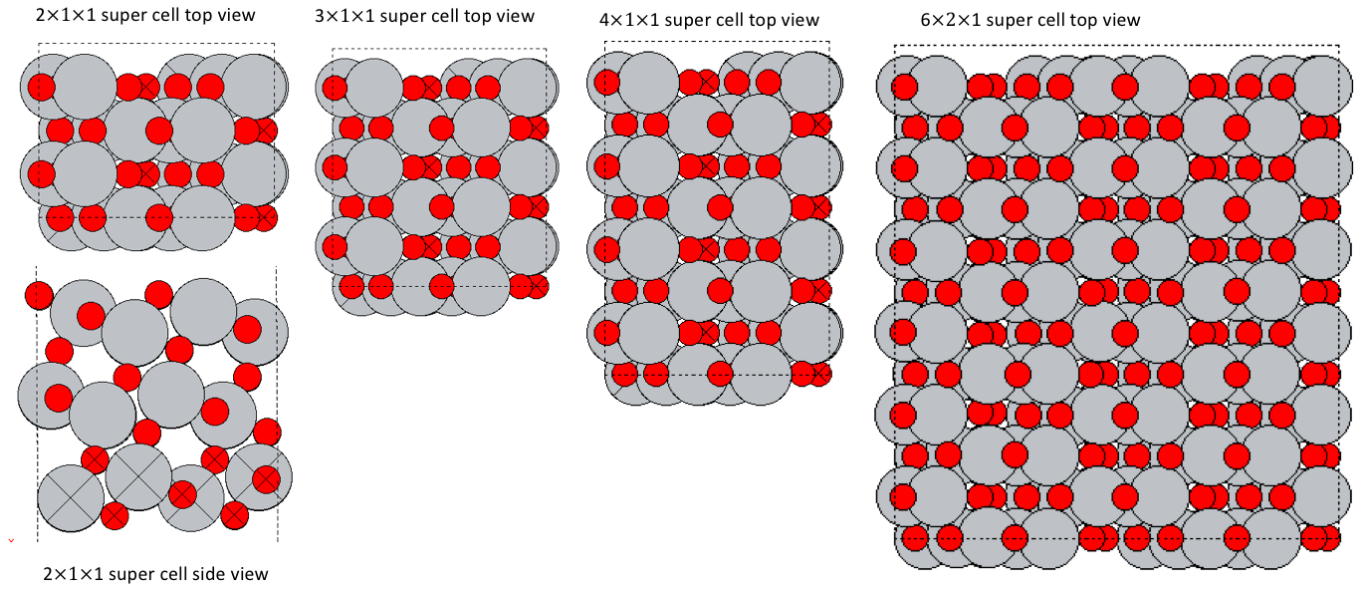


FIG. 2. Different super cell size of surfaces used in all the calculations.

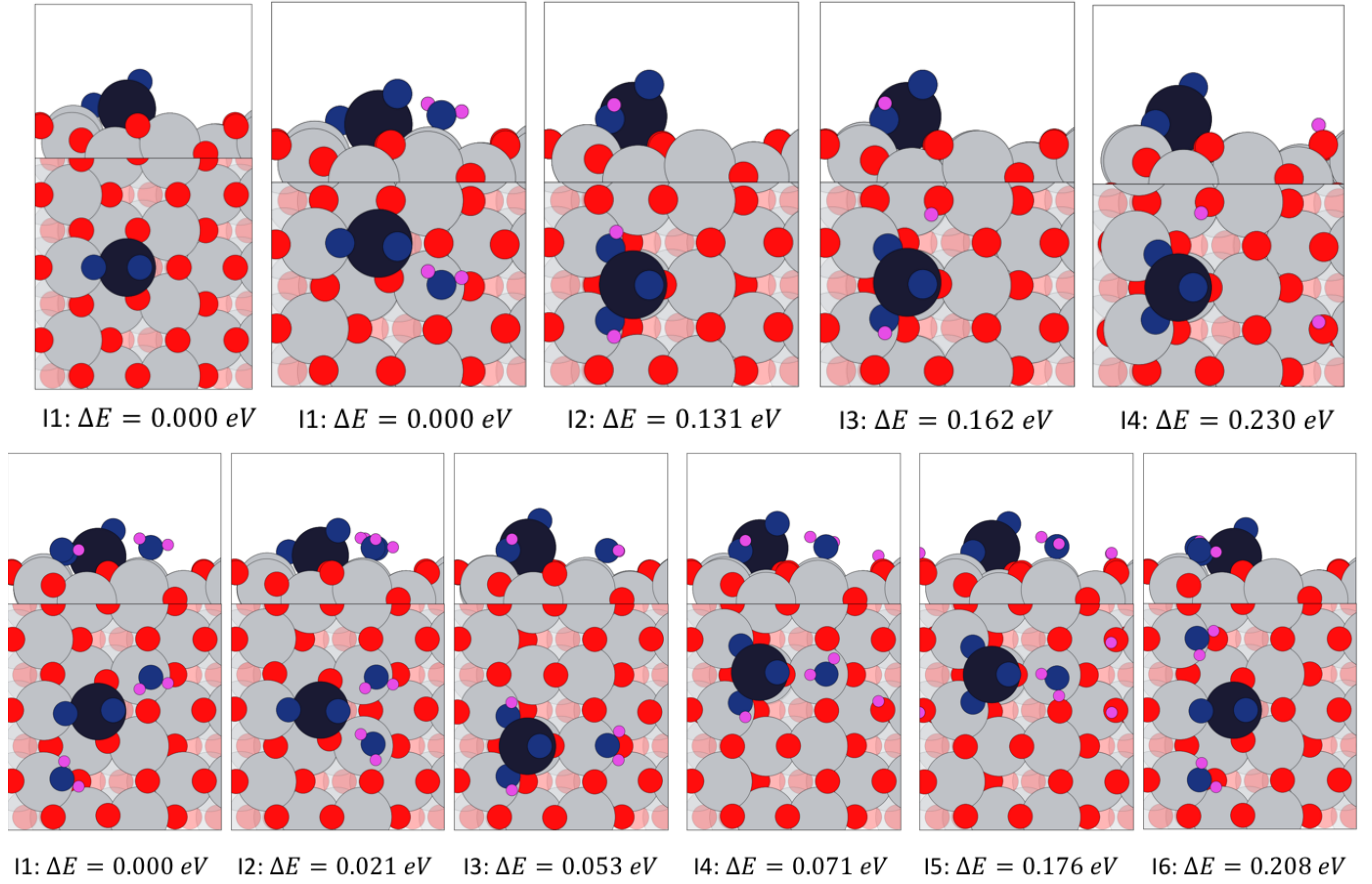


FIG. 3. All the possible low-lying isomers found for VO_2 , $\text{VO}_2\text{H}_2\text{O}$ and $\text{VO}_22\text{H}_2\text{O}$ clusters with GOFEE were DFT relaxed with one Oxygen vacancy created in 2nd layer. Here two types of super cell sizes were used those are $2 \times 1 \times 1$ super cell for VO_2 , $\text{VO}_2\text{H}_2\text{O}$ and $3 \times 1 \times 1$ super cell for $\text{VO}_22\text{H}_2\text{O}$ clusters.

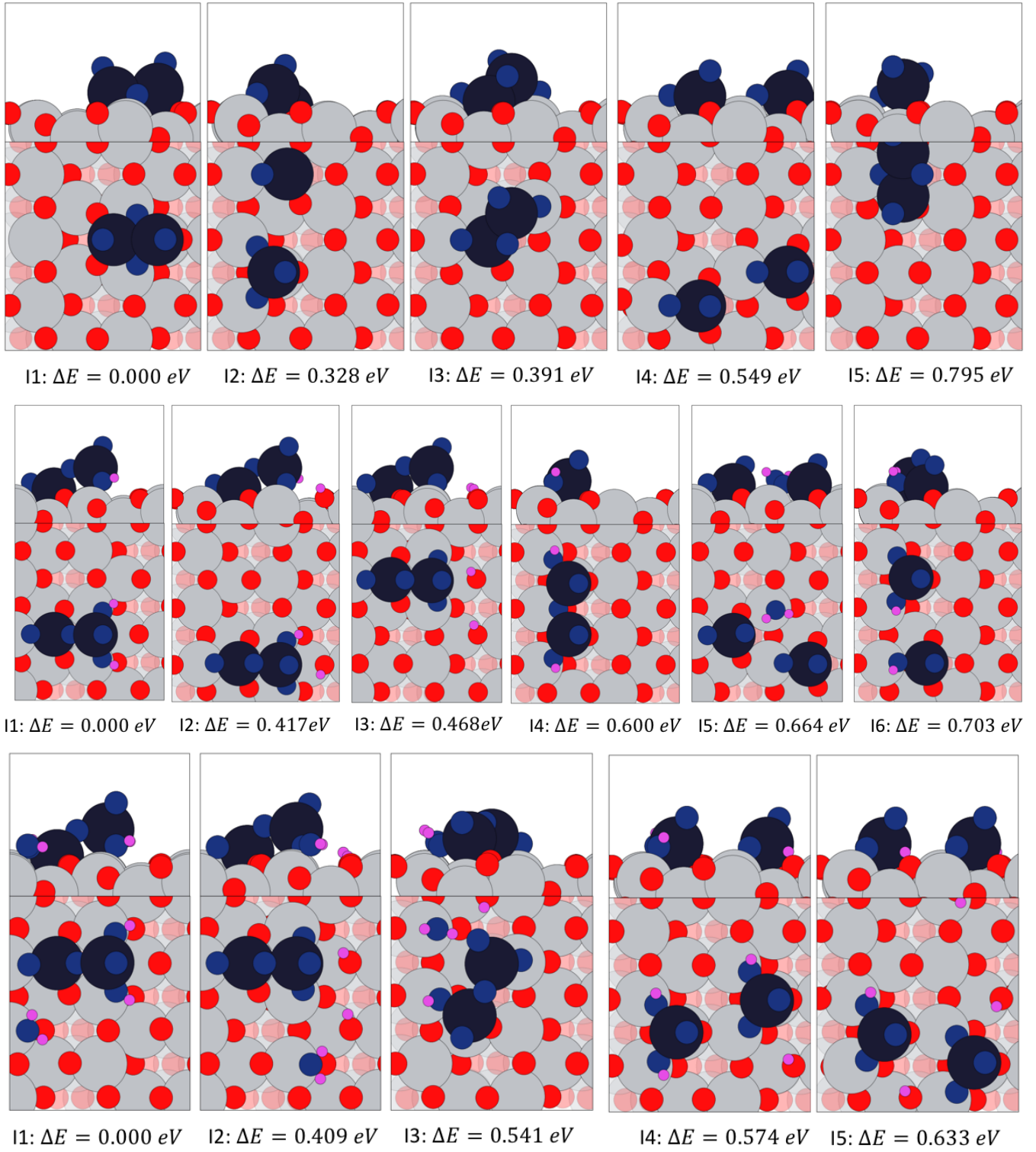


FIG. 4. All the possible low-lying isomers found for V_2O_4 , $\text{V}_2\text{O}_4 \cdot \text{H}_2\text{O}$ and $\text{V}_2\text{O}_4 \cdot 2\text{H}_2\text{O}$ clusters with GOFEE were DFT relaxed with one Oxygen vacancy created in 2nd layer. Here $3 \times 1 \times 1$ super cell used for all clusters.

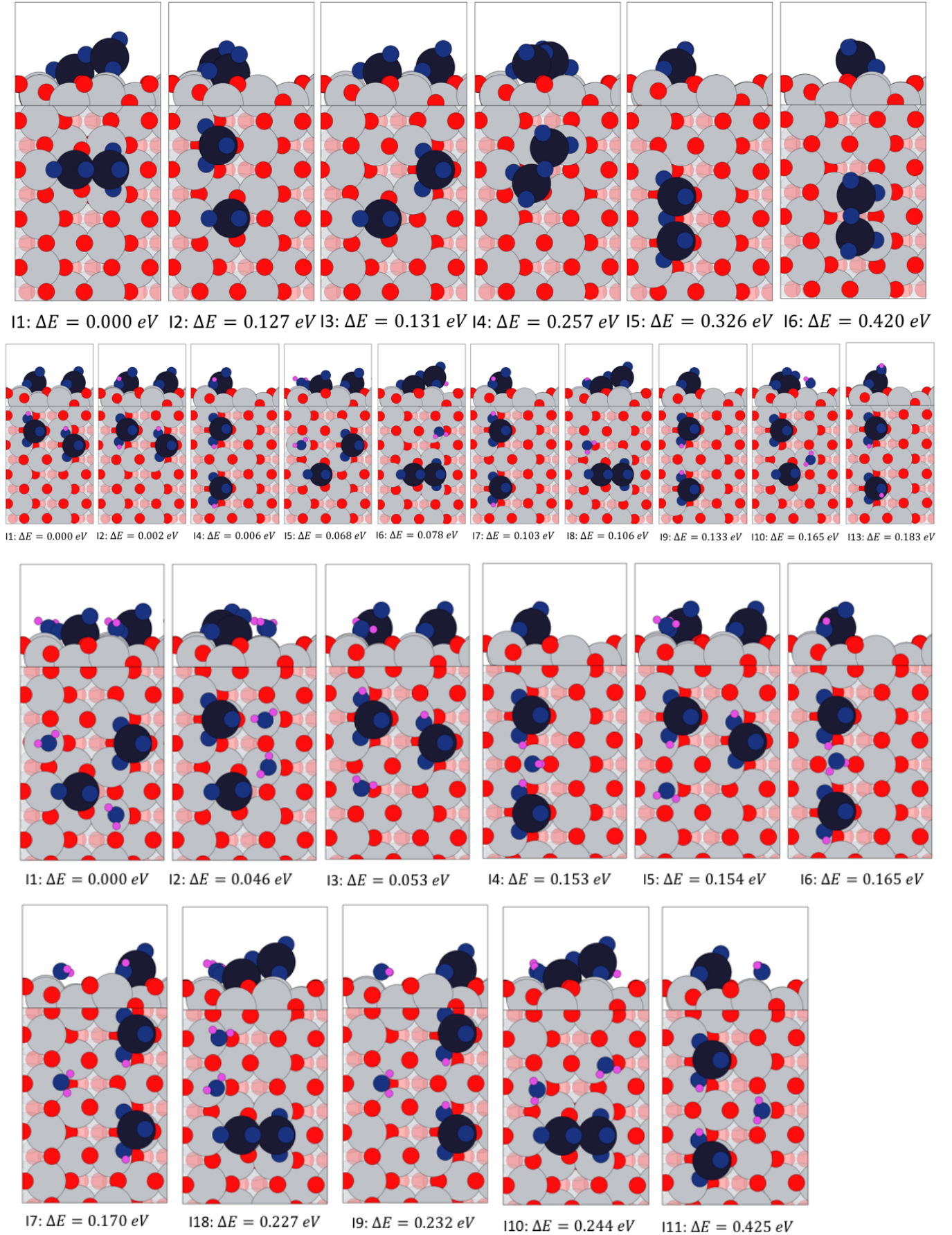


FIG. 5. All the possible low-lying isomers found for V_2O_5 , $\text{V}_2\text{O}_5 \cdot \text{H}_2\text{O}$ and $\text{V}_2\text{O}_5 \cdot 2\text{H}_2\text{O}$ clusters with GOFEE were DFT relaxed with one Oxygen vacancy created in 2nd layer. Here $4 \times 1 \times 1$ super cell used for all clusters.

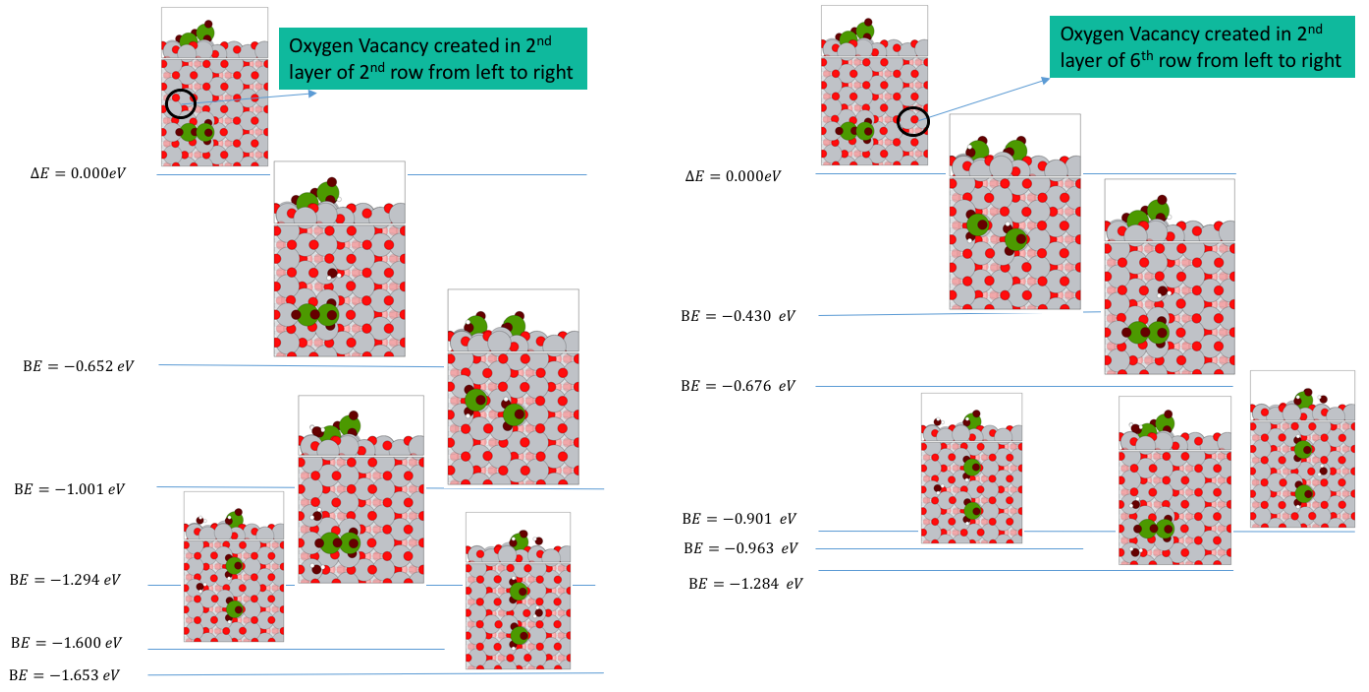


FIG. 6. Binding energy order for best structures of V_2O_5 , $\text{V}_2\text{O}_5 \cdot \text{H}_2\text{O}$ and $\text{V}_2\text{O}_5 \cdot 2\text{H}_2\text{O}$ clusters found in global optimization were re-optimised with $6 \times 2 \times 1$ super cell and two different positions of oxygen vacancy created.

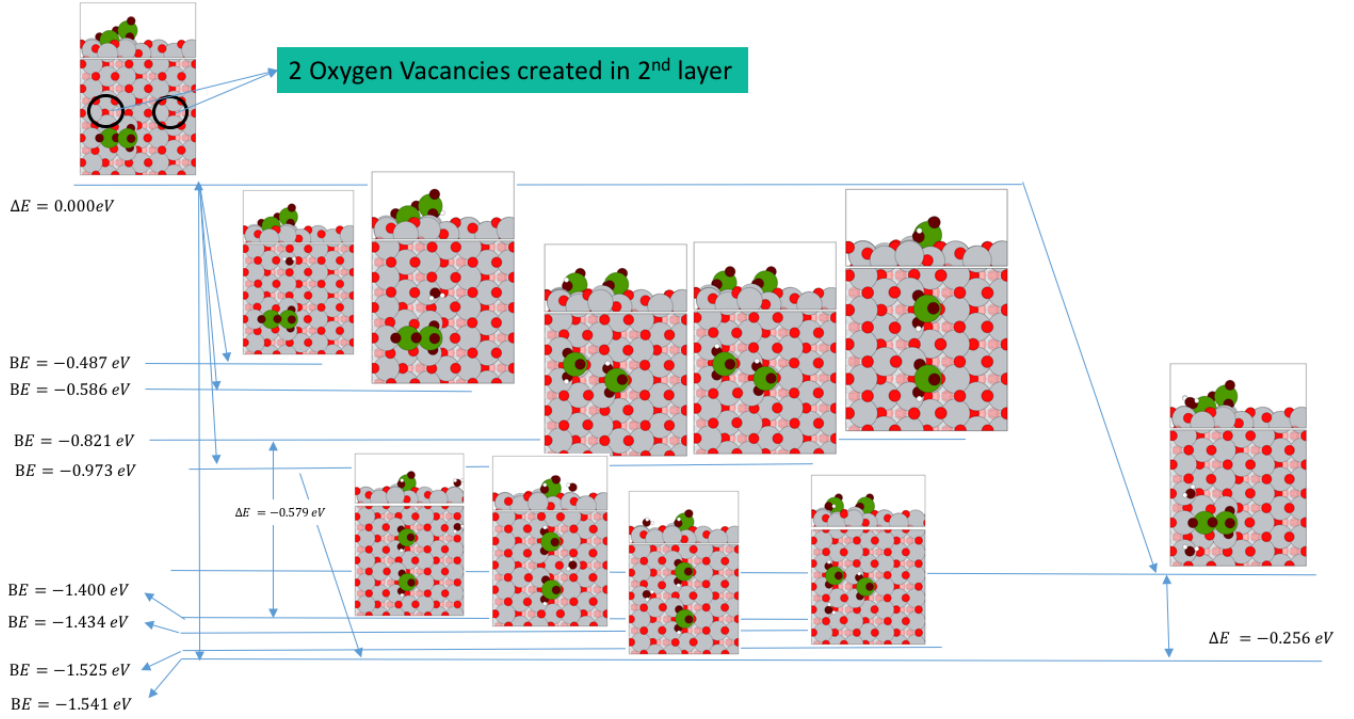


FIG. 7. Binding energy order for best structures of V_2O_5 , $\text{V}_2\text{O}_5 \cdot \text{H}_2\text{O}$ and $\text{V}_2\text{O}_5 \cdot 2\text{H}_2\text{O}$ clusters found in global optimization were re-optimised with $6 \times 2 \times 1$ super cell and two oxygen vacancy created.