|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Structure | E\_DFT (eV) |  | BE (eV)= E((2 H2O + V2O5)/TiO2(101))  -(V2O5)/TiO2(101)  -2 H2O |  |
| H2O | -14.0422116 | 2\* H2O = -28.08442 |  |  |
| (2 H2O + V2O5)/TiO2(101)  (I1) | -986.162322 |  | -1.880 |  |
| (V2O5)/TiO2(101)  (I1) | -956.1959906 |  |  |  |
| (2 H2O + V2O5)/TiO2(101)  (I3) | -986.096505 |  | -1.844 |  |
| (V2O5)/TiO2(101)  (I3) | -956.167686 |  |  |  |
| (1 H2O + V2O5)/TiO2(101)  (I2) | -971.2640038 |  | -0.897 |  |
| ( V2O5)/TiO2(101)  (I2) | -956.3244426 |  |  |  |
| (1 H2O + V2O5)/TiO2(101)  (I6) | -971.1661978 |  | -0.927 |  |
| ( V2O5)/TiO2(101)  (I6) | -956.19635 |  |  |  |
| (1 H2O + V2O5)/TiO2(101)  (I8) | -971.057496 |  | -0.817 |  |
| (V2O5)/TiO2(101)  (I8) | -956.1972986 |  |  |  |
| (1 H2O + V2O5)/TiO2(101)  (I37) | -970.9680407 |  | -0.758 |  |
| (V2O5)/TiO2(101)  (I37) | -956.167738 |  |  |  |
| (1 H2O + V2O5)/TiO2(101)  (I44) | -970.889305 |  | -0.679 |  |
| (V2O5)/TiO2(101)  (I44) | -956.167116 |  |  |  |