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Oxygen Alignment Energy at Water Splitting

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Abstract: *The oxygen alignment energy has been calculated and compared with the water splitting energy.*

Keywords: *oxygen alignment energy, water splitting energy*

1. Introduction

Let us calculate the oxygen alignment energy and compare it with the water splitting energy.

2. The Alignment Energy

The alignment energy of the atom or molecule is a concept where the kinetic energy of the electron enables the alignment of the electron with its atom or molecule nature [1], [2], [3] and [4]. It is given by the next formula:

$$Wk_{alignment} = \left(\frac{R_{unaligned}}{R_{aligned}} - 1\right) m_{electron}^{rest} c^2. \quad (1)$$

Where $R_{unaligned}$ is the unaligned modified ratio of atom or molecule mass to electron mass:

$$R_{unaligned} = \frac{m_{atom\ or\ molecule}}{m_{electron}^{rest}}\ s(1). \quad (2)$$

The factor $s(1) = 1{,}696\ 685\ 529\ ...$ is the average elliptic-hyperbolic unit expressed in Compton wavelengths of the electron given for $n = 1$ by the next equation:

$$s(n) = n\left(2 - \frac{1}{\sqrt{1 + \frac{\pi^2}{n^2}}}\right), \qquad n \in \mathbb{N}. \quad (3)$$

And the aligned modified ratio $R_{aligned}$ is approximately the down rounded whole value of the unaligned modified ratio $R_{unaligned}$:

$$R_{aligned} = s\left(\text{ROUNDDOWN}\left(R_{unaligned}\right)\right) \approx \text{ROUNDDOWN}\left(R_{unaligned}\right). \quad (4)$$

Using the data from the reference [5] and applying the equations (1), (2), (3) the practically identical alignment energies of the oxygen atom O and molecule O_2 have been calculated. The oxygen alignment characteristics are presented in Table 1.

Table1. *The alignment characteristics of oxygen atom O and molecule O_2*

Oxygen	Mass (Da)	Unaligned R	Aligned R	Alignment energy (eV)
O	15,994915	49470,16901	49470,00010	1,745
O2	31,989830	98940,33802	98940,00005	1,746
e^-	0,00054857990907			

3. The Water Splitting Energy

The process of water splitting is highly endothermic and requires a Gibbs free energy of 2,46 eV per molecule at T=25°C and p=100 kPa [6]. Because of two electrons involved in the redox reaction the

energy of 1,23 eV per electron is needed which corresponds to light with a wavelength of 1008 nm:

$$H_2O \xrightarrow{\lambda_{light}=1008\ nm} H_2 + \frac{1}{2}O_2. \quad (5)$$

The redox reaction on the surface of the photocatalyst is described by the following steps [6]:

Oxidation:

$$H_2O - 2e^- \rightarrow 2H^+ + \frac{1}{2}O_2. \quad (6)$$

($-e^- = h^+$)

And reduction:

$$2H^+ + 2e^- \rightarrow H_2. \quad (7)$$

This means that the photocatalyst must have a bandgap > 1,23 eV, or else the electrons will not have enough energy to start the reaction [6]. In practice, this limit should be 1,6 eV to 1,8 eV due to some overpotentials [7].

4. The Minimal Theoretical and Minimal Real Bandgap

Let us try with the help of oxygen alignment energy to explain the discrepancy between the minimal theoretical and minimal real bandgap. Indeed, the oxygen alignment energy of 1,75 eV (Table 1) is within the suggested minimal real bandgap range: 1,6 eV < 1,75 eV < 1,8 eV. One can propose that the minimal theoretical bandgap energy of 1,23 eV is enough only for the splitting of water to the unaligned oxygen. And the minimal real bandgap energy of 1,75 eV is needed for the formation of aligned oxygen to supress the reverse reaction of formation the water from hydrogen and oxygen again. Details of photocatalytic water splitting are shown in Figure 1. [8].

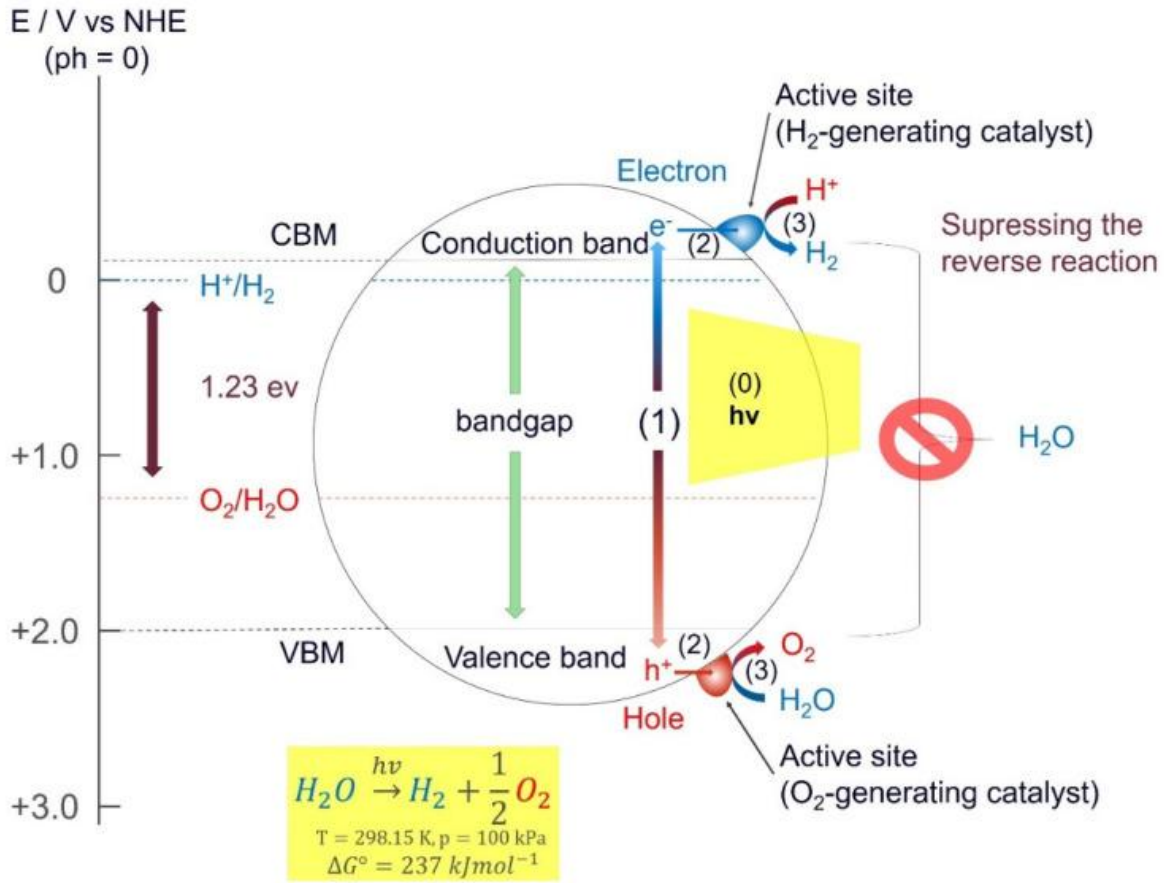

Figure1. *Schematic illustration of the main photocatalytic steps for a semiconductor photocatalyst [8]. (1) light is absorbed to generate electron–hole pairs; (2) migration of excited carriers (electrons e^- and holes h^+) to the surface; (3) surface reaction to produce hydrogen with electrons and oxygen with holes;* 🚫 *bandgap to supress the reverse reaction.*

5. INSTEAD OF CONCLUSION

The explanation of needed minimal overpotential energy of 0,52 eV at water splitting is offered:

$$W_{overpotential} = W_{alignment} - G^0 per\ electron = 1{,}75\ eV - 1{,}23\ eV = 0{,}52\ eV. \quad (8)$$

DEDICATION

To my granddaughter Noemi and the miracle of life. Toronto, July 26, 2021

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