Alignment Energy Role in Water Formation

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Abstract: *The alignment energy change of the oxygen electrons coincides with the activation energy of water formation on the uncovered (0001) facet of ruthenium*

Keywords: *Alignment energy of water and its constituents, activation energy of water formation*

1. INTRODUCTION

The alignment energy enables the internalization of the electron with the physicochemical nature of the world to which the electron belongs [1]. In this fragment we will show how the change in alignment energy is reflected in the formation of water:

$$2H_2 + O_2 \rightarrow 2H_2O. \tag{1}$$

2. ALIGNMENT CHARACTERISTICS OF WATER AND ITS CONSTITUENTS

The alignment characteristics of water H_2O and its constituents H, H_2, O, O_2, OH as well as electron itself (e^-) are presented in Table1. Masses of the elements (H, O) and e^- are taken from reference [2] and [3], respectively.

Table1. *The alignment characteristics of H, H_2, O, O_2, OH, H_2O and e^-*

Particle	Mass (Da)	$R_{unaligned} = \dfrac{m_{particle}}{m_{e^-}} s(1)$	$n \in \mathbb{N}$	$R_{aligned} = s(n) = n\left(2 - \dfrac{1}{\sqrt{1+\frac{\pi^2}{n^2}}}\right)$	$W_{alignment} = \left(\dfrac{R_{unaligned}}{R_{aligned}} - 1\right) m_{electron} c^2$
H	1,007825031898	3117,07031	3117	3117,00158	11,2671 eV
H_2	2,015650063796	6234,14062	6234	6234,00079	11,4617 eV
O	15,994914619257	49470,16783	49470	49470,00010	1,7326 eV
O_2	31,989829238514	98940,33567	98940	98940,00005	1,7334 eV
OH	17,002739651155	52587,23814	52587	52587,00009	2,3132 eV
H_2O	18,010564683053	55704,30845	55704	55704,00009	2,8288 eV
e^-	0,00054857990907	s(1)=1,69668…	1	s(1)	0 eV

The alignment energy maintains the physicochemical nature of part (electron) as a constituent of whole (atom, molecule). The electron as a part of itself has an empty whole nature for which no alignment energy is needed. The presented physicochemical entities in our case show that homogenous molecules (H_2, O_2) have higher alignment energy than the atoms (H, O) from which they emanate :

$$W_{H_2}^{alignment} = 11{,}4617 \, eV > W_H^{alignment} = 11{,}2671 \, eV . \tag{2a}$$

$$W_{O_2}^{alignment} = 1,7334 \ eV > W_O^{alignment} = 1,7326 \ eV \ . \tag{2b}$$

And heterogeneous entities (OH, H$_2$O) have the alignment energy lying inside the interval determined by their constituents (H, O):

$$W_H^{alignment} = 11,2671 \ eV > W_{OH}^{alignment} = 2,3132 \ eV > W_O^{alignment} = 1,7326 \ eV. \tag{3a}$$

$$W_H^{alignment} = 11,2671 \ eV > W_{H_2O}^{alignment} = 2,8288 \ eV > W_O^{alignment} = 1,7326 \ eV. \tag{3b}$$

The replacement of the electron physicochemical nature is accompanied by a change in the alignment energy. For instance, in water formation a part of the hydrogen alignment energy should be released and a part of the oxygen alignment energy invested. And the latter could play the role of activation energy in the formation of water. The alignment energy difference of the electron in water and its constituents are collected in Table2.

Table2. *The alignment energy difference between electron e⁻ in different physicochemical entities H, H₂, O, O₂, OH, H₂O and e⁻ itself*

Alignment energy difference (eV)	→ H	→ H$_2$	→ O	→ O$_2$	→ **OH**	→ H$_2$O	→ e^-
H →	0	0,1946	-9,5345	-9,5337	-8,9539	-8,4383	-11,2671
H$_2$ →	-0,1946	0	-9,7291	-9,7283	-9,1485	-8,6329	-11,4617
O →	+9,5345	+9,7291	0	+0,0008	**+0,5806**	+1,0962	-1,7326
O$_2$ →	+9,5337	+9,7283	-0,0008	0	+0,5798	+1,0954	-1,7334
OH →	+8,9539	+9,1485	-0,5806	-0,5798	0	+0,5156	-2,3132
H$_2$O →	+8,4383	+8,6329	-1,0962	-1,0954	-0,5156	0	-2,8288
e^- →	+11,2671	+11,4617	+1,7326	+1,7334	+2,3132	+2,8288	0

From Table 2 we can see that the easiest way to achieve H$_2$O is the step by step formation of water molecule:

$$O_2 \rightarrow O \rightarrow OH \rightarrow H_2O. \tag{4}$$

The electron from being a part of an O$_2$ molecule should in the first step become a part of the O atom:

$$W_{O_2 \rightarrow O}^{alignment} = -0,0008 \ eV \ ... In \ this \ step \ the \ energy \ is \ released. \tag{4a}$$

The electron from being a part of an O atom should in the second step become a part of the OH entity:

$$W_{O \rightarrow OH}^{alignment} = 0,5806 \ eV \ ... In \ this \ step \ the \ energy \ is \ invested. \tag{4b}$$

The electron from being a part of an OH entity should in the third step become a part of the H$_2$O molecule:

$$W_{OH \rightarrow H_2O}^{alignment} = 0,5156 \ eV \ ... In \ this \ step \ the \ energy \ is \ invested. \tag{4c}$$

The energy (4b) as the highest invested energy could play a role of the activation energy of water formation:

$$W_{activation}^{H+O \rightleftharpoons OH} = 0,5806 \ eV. \tag{5}$$

3. WATER FORMATION ON THE RUTHENIUM SURFACE RU(0001)

In principle, the following reaction steps can lead to water formation on the (0001) facet of ruthenium, denoted Ru(0001) [4]:

$$H_{2(g)} \rightleftharpoons 2H_{(ads)}. \tag{6a}$$

$$\boldsymbol{H_{(ads)} + O_{(ads)} \rightleftharpoons OH_{(ads)}.} \tag{6b}$$

$$OH_{(ads)} + H_{(ads)} \rightleftharpoons H_2O_{(ads)}. \tag{6c}$$

$$2OH_{(ads)} \rightleftharpoons H_2O_{(ads)} + O_{(ads)}. \tag{6d}$$

$$H_2O_{(ads)} \rightleftharpoons H_2O_{(g)}. \tag{6e}$$

On uncovered Ru(0001), reactions (6a)–(6c) and (6e) have been described as part of the water formation mechanism, with reaction (6b) being the rate-determining step [5] possessing the activation energy yielding a value of 0.59±0.04 eV by the Arrhenius analysis [4]:

$$E_{activation}^{H+O\rightleftharpoons OH} = 0{,}59 \pm 0.04 \; eV. \tag{7}$$

4. RESULT

The activation energy of water formation as a consequence of alignment concept, denoted $W_{activation}^{H+O\rightleftharpoons OH}$ (5), coincides with the activation energy of water formation on the uncovered Ru(0001), denoted $E_{activation}^{H+O\rightleftharpoons OH}$ (7):

$$W_{activation}^{H+O\rightleftharpoons OH} \approx E_{activation}^{H+O\rightleftharpoons OH}. \tag{8a}$$

Since

$$0{,}5806 \; eV \in 0{,}59 \pm 0{,}04 \; eV. \tag{8b}$$

5. CONCLUSION

Figure1. *Equality [6]*

DEDICATION

To providence but against prejudice

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ADDENDUM

At water formation in a physically confined space under silica thin films approximately twice lower activation energy was observed than on the uncovered Ru(0001) surface [4]:

$$E_{activation}^{covered \; Ru} = 0.27 \pm 0.02 \; eV < E_{activation}^{uncovered \; Ru} = 0.59 \pm 0.04 \; eV. \tag{9}$$

One of the possible explanations was offered that in the confined space the reaction (6d) could become the rate-determining step. Our concept does not support such option since the mentioned step is not accompanied with enough low change in the alignment energy:

$$W_{2OH \rightarrow H_2O}^{alignment} = 0{,}5156 \; eV \neq E_{activation}^{covered \; Ru} = 0.27 \pm 0.02 \; eV. \tag{10}$$

Other explanations should take precedence. For instance, let us propose one step water formation:

$$2H_{(ads)} + O_{(ads)} \rightleftharpoons H_2O. \tag{11}$$

Here the electron from being a part of an O entity in one step becomes a part of the H_2O molecule. For this purpose the next alignment energy need to be invested (see Table 2):

$$W_{O \to H_2O}^{alignment} = 1{,}0962 \ eV. \tag{12a}$$

In the confined space on Ru(0001) surface under silica thin films 4-times splitting such alignment energy comes into play as an activation energy in water formation:

$$E_{activation}^{covered \ Ru} = \frac{1{,}0962 \ eV}{4} \in 0{,}27 \ \pm 0.02 eV. \tag{12b}$$