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# The Hydrated-electron Absorption Spectrum in the View of the Band Theory of Liquid Water

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**ABSTRACT**

At photo-ionization of liquid water, its inherent species such as hydroxonium cation and hydroxide anion are considered in the band theory as electron acceptor and its donor respectively with forming their excited radicals. In this case, there are also other carriers for hydrated electrons and holes like negatively and positively onecharged molecular pairs that are nonequilibrium to each other and in attitude to mentioned radicals. Here offered model of 4 electron transitions between these natural species gives good consent with the experimental data for absorption spectrum of hydrated electrons in the bulk of liquid water.

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## Introduction

It is known that the hydrated electron is the simplest quantum species in liquid water. Its absorption spectrum is characterized by a broad, asymmetric, and featureless optical band with a Gaussian function on the lowenergy side from the maximum, and with the Lorentzian function on the high-energy one as a "blue tail" of the spectrum [1,2].

Despite five decades of studying hydrated electrons, their physical nature is not still understood. All researchers have concentrated their attention on the quantum theory of oneelectron excitations in a hollow sphere which describes the excited hydrated-electron inside or outside of a molecular cavity [2-5].

At the same time, the hydrated electron in real dynamic state in water turns out to be built into the structure of hydrogen bonds of water what is following from the solvation model supported by various experiments [4].

In addition, the observed "blue tail" of the hydrated-electron absorption spectrum is to be a contribution of many quantum states of electron in the hollow quasi-sphere [2,5]. This seems doubtful due to comparatively the long time of the hydrated-electron absorption in reality. Therefore such electron can be considered simultaneously in cavity, on neighboring water molecules, and in tail of hydrogen bonds [6]. It is shown that all three of these contributions are significant and important for description of the hydrated electron having the complex nature, and oversimplified interpretations based on pseudo-potential models are wrong. Then, we can suggest that the behavior of hydrated electron in bulk water is conditioned mainly by its properties of the condensed matter.

We offer to use the electronic band theory of liquid dielectrics in order to clarify these issues of the hydrated electron [7]. We believe that the excited hydrated electron is in one of two allowed energy levels in the band gap of liquid water. The molecular carriers of these occupied levels are the hydroxonium radical $H_3O$ and its cluster with hydride anion $H_3O \cdot OH^-$ which is the one-charged molecular pair $(H_2O)^-_2$ [8-13]. The hydrogen bonds of these carriers with other molecules of water extend in a spatial domain with a sufficiently large radius of gyration for the hydrated electron.

## The Correction of Band Structure of Liquid Water

Earlier, we have suggested that the band gap of liquid water (~6.9 eV) contains the allowed local electron levels that lie symmetrically to the middle of band gap which is Fermi level $\varepsilon_F$ of stoichiometric water $H_2O$ as shown in Figure 1a [9,14]. The molecular carriers of these electron levels are the inherent species in liquid water: the occupied-by-electron hydroxide $OH^-$ and the vacant hydroxonium $H_3O^+$ that are being generated by the reaction of dissociation

$$2H_2O \leftrightarrow H_3O+ + OH^- \qquad (1)$$

and their mole fractions $[H_3O^+]$ and $[OH^-]$ satisfy the ratio

$$[H_3O^+] \cdot [OH^-] = K_w \qquad (2)$$

with the dissociation constant $K_w = 10^{-15}$ M$^2$ at $T = 274$K [15,16].

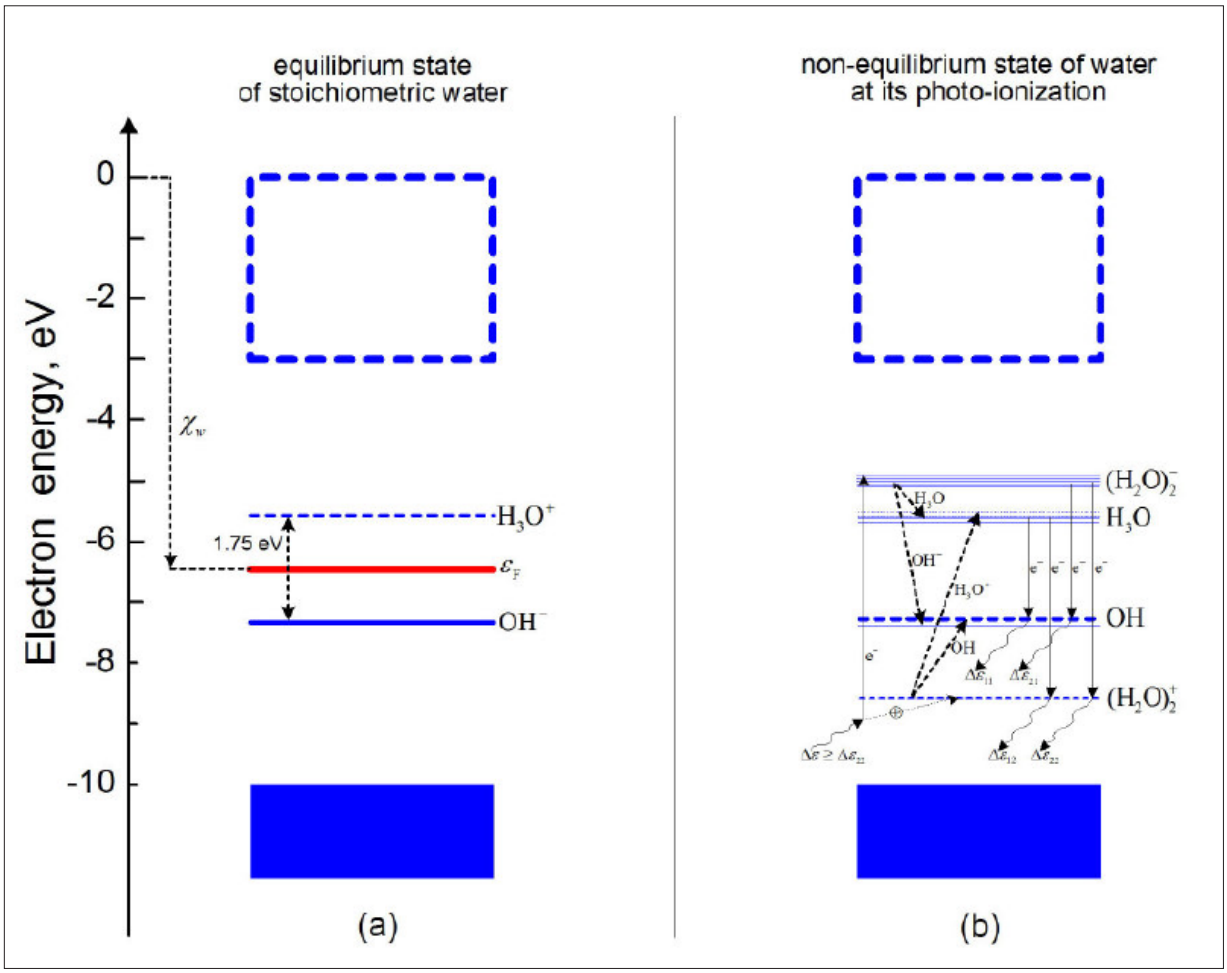


Figure 1: The band structure of liquid water: a) the equilibrium state with two allowed local electron levels, the first is the occupied-by-electron hydroxyl $OH^-$ (blue full line) and the second is the vacant hydroxonium $H_3O^+$ (blue dotted line) with the energy difference between them of 1.75 eV [9]; these levels lie symmetrically to the middle of band gap which is Fermi level $\varepsilon_F$ of stoichiometric water, $\chi_w$ is its work function equal to 6.45 eV [14]; b) the non-equilibrium state of water with excited hydrated electrons in the levels $(H_2O)^-_2$ and $H_3O$ (blue full lines), with vacant levels of $(H_2O)^+_2$ and OH (blue dotted lines) as two ground states; the black wave arrows are quanta of light with energy $\Delta\varepsilon_{ik}$ where "*i*" is the excited level and "*k*" is the ground level, the thin black arrows are electron transitions, $\oplus$ denotes the water molecule without electron, and the black dotted arrows denote brownian decay (without radiation) of $(H_2O)^-_2$ and $(H_2O)^+_2$ into inherent species, shown by Eq. (3) and (4).

In the case of water photo-ionization, hydrated electrons have a recombination time less 10 μs [17]. The mechanism responsible for this effect is so-called scavenging process, whereby an electron recombines with one of the ions of the donor molecules or another scavenger in the aqueous solution [18].

One can see in Figure 1b that the all electron states are non-equilibrium because electrons are in the upper energy levels $(H_2O)^-_2$ and $H_3O$ whereas the low levels OH and $(H_2O)^+_2$ are vacant as holes. The last species is the built-up one ($H_3O^+$· OH) [12].

Obviously, the electrons in upper species are excited not only relative to the lower ones but between themselves due to diffusive decay of $(H_2O)^-_2$ by means of the reaction:

$$(H_2O)_2^- \rightarrow H_3O + OH^-, \qquad (3)$$

which is modeled by a simple equation of balance in a spatial area with large gyration radius that can be considered equal for these species [18]. Therefore the energy difference between them has to be less than the same for the second pair: OH and $(H_2O)^+_2$ with the small gyration radius and the reaction of decay

$$(H_2O_2)^+_2 \rightarrow H_3O^+ + OH \qquad (4)$$

Consequently, the energy dispersion of electron levels is also equal in the every case: $\sigma_1^- = \sigma_2^- = \sigma^-$ for the pair $H_3O$, $(H_2O)^-_2$ and $\sigma_1^+ = \sigma_2^+ = \sigma^+$ for OH, $(H_2O)^+_2$ but $\sigma^+ << \sigma^-$ (see Figure 1b).

The absorption spectrum of hydrated electrons out of the levels: $(H_2O)^-_2$ and $H_3O$ is determined by the sum $\sum_{i=1}^{2}\sum_{k=1}^{2} p_{ik}$ of their transition probabilities $P_{ik}$ into two ground levels: OH and $(H_2O)^+_2$.

$$\left.\begin{aligned} &H_3O + OH \xrightarrow{e^-} H_3O^+ + OH^- && (p_{11})\\ &H_3O + (H_2O)_2^+ \xrightarrow{e^-} H_3O^+ + 2H_2O && (p_{12})\\ &(H_2O)_2^- + OH \xrightarrow{e^-} 2H_2O + OH^- && (p_{21})\\ &(H_2O)_2^- + (H_2O)_2^+ \xrightarrow{e^-} 4H_2O && (p_{22}) \end{aligned}\right\} \qquad (5)$$

Here, $P_{ik}$ denotes the probability of electron transition out of the excited level "*i*" into the ground level "*k*".

**The Calculation of Absorption Spectrum**

We can use the Gaussian function [19]

$$g(\varepsilon)=\frac{1}{\sigma\sqrt{2\pi}}\exp(-\frac{(\varepsilon-\mu)^2}{2\sigma^2}) \qquad (6)$$

with the condition $\int_{\mu-\infty}^{\mu+\infty} g(x)dx=1$ for the normal distribution of electrons energy in species: $H_3O$, $(H_2O)^-_2$ and the holes energy in the species: OH, $(H_2O)_2^+$. Here, $\varepsilon$ is their energy near the equilibrium level $\mu$, $\sigma$ is the energy dispersion of normal distribution for these particles.

In this case, the normal distribution is caused by the thermal fluctuations $k_BT$ of liquid water. Therefore one can naturally accept: $\sigma^+=k_BT/3$. Then, we can introduce the normalized Gaussian functions:

$$\left.\begin{aligned} g(\varepsilon_1^-)&=\frac{1-\alpha^-}{\sigma^-\sqrt{2\pi}}\exp(-\frac{(\varepsilon_1^--\mu_1^-)^2}{2\sigma^{-2}})\\ g(\varepsilon_2^-)&=\frac{\alpha^-}{\sigma^-\sqrt{2\pi}}\exp(-\frac{(\varepsilon_2^--\mu_2^-)^2}{2\sigma^{-2}})\\ g(\varepsilon_1^+)&=\frac{1-\alpha^+}{\sigma^+\sqrt{2\pi}}\exp(-\frac{(\varepsilon_1^+-\mu_1^+)^2}{2\sigma^{+2}})\\ g(\varepsilon_2^+)&=\frac{\alpha^+}{\sigma^+\sqrt{2\pi}}\exp(-\frac{(\varepsilon_2^+-\mu_2^+)^2}{2\sigma^{+2}}) \end{aligned}\right\} \qquad (7)$$

for two populated-by-electrons energy levels $\mu^-_1 < \mu^-_2$ of the hydroxonium radical $H_3O$ and charged molecular pair $(H_2O)^-_2$ respectively as well as for the vacant levels $\mu^+_2 < \mu^+_1$ of the hydroxyl radical OH and the hydrated "hole" $(H_2O)^+_2$ respectively with $\mu^-_1 < \mu^+_1 = 1.75$ eV (see Figure 1b) [9]. Here

$$\alpha^-=\frac{\exp(s^--\frac{\delta^-}{k_BT})}{1+\exp(s^--\frac{\delta^-}{k_BT})} \qquad \alpha^+=\frac{\exp(s^+-\frac{\delta^+}{k_BT})}{1+\exp(s^+-\frac{\delta^+}{k_BT})}$$

$s^- >> 1$, $s^+ >> 1$ are the entropies of transition (3) and (4) respectively without radiation and one-charged molecular pairs $(H_2O)^-_2$ $(H_2O)^+_2$ have electron energies relative to radicals:

$\delta^-=\mu^-_2-\mu^-_1>0$ and $\delta^+=\mu^+_1-\mu^+_2>0$; $k_B$ is the Boltzmann constant; $T$ is Kelvin temperature.

Now, one can obtain the partial probability $p_{ik}(\Delta\varepsilon)$ of electron transition out of the populated level "$i$" into the vacant one "$k$" as a function of radiation energy $\Delta\varepsilon$ :

$$\begin{aligned} p_{11}(\Delta\varepsilon)&=\int_{\mu_1^+-3\sigma^+}^{\mu_1^++3\sigma^+} g(\varepsilon_1^+)d\varepsilon_1^+\int_{\mu_1^--3\sigma^-}^{\mu_1^-+3\sigma^-} g(\varepsilon_1^-)\delta(\varepsilon_1^--\varepsilon_1^+-\Delta\varepsilon)d\varepsilon_1^-\\ &=\frac{\nu_{11}}{2\pi\sigma^-\sigma^+}\int_{\mu_1^+-3\sigma^+}^{\mu_1^++3\sigma^+}\exp[-\frac{(\varepsilon_1^+-\mu_1^+)^2}{2\sigma^{+2}}-\frac{(\varepsilon_1^++\Delta\varepsilon-\mu_1^-)^2}{2\sigma^{-2}}]d\varepsilon_1^+, \end{aligned} \qquad (8)$$

$$\begin{aligned} p_{12}(\Delta\varepsilon)&=\int_{\mu_2^+-3\sigma^+}^{\mu_2^++3\sigma^+} g(\varepsilon_2^+)d\varepsilon_2^+\int_{\mu_1^--3\sigma^-}^{\mu_1^-+3\sigma^-} g(\varepsilon_1^-)\delta(\varepsilon_1^--\varepsilon_2^+-\Delta\varepsilon)d\varepsilon_1^-\\ &=\frac{\nu_{12}}{2\pi\sigma^-\sigma^+}\int_{\mu_2^+-3\sigma^+}^{\mu_2^++3\sigma^+}\exp[-\frac{(\varepsilon_2^+-\mu_2^+)^2}{2\sigma^{+2}}-\frac{(\varepsilon_2^++\Delta\varepsilon-\mu_1^-)^2}{2\sigma^{-2}}]d\varepsilon_2^+, \end{aligned} \qquad (9)$$

$$\begin{aligned} p_{21}(\Delta\varepsilon)&=\int_{\mu_1^+-3\sigma^+}^{\mu_1^++3\sigma^+} g(\varepsilon_1^+)d\varepsilon_1^+\int_{\mu_2^--3\sigma^-}^{\mu_2^-+3\sigma^-} g(\varepsilon_2^-)\delta(\varepsilon_2^--\varepsilon_1^+-\Delta\varepsilon)d\varepsilon_2^-\\ &=\frac{\nu_{21}}{2\pi\sigma^-\sigma^+}\int_{\mu_1^+-3\sigma^+}^{\mu_1^++3\sigma^+}\exp[-\frac{(\varepsilon_1^+-\mu_1^+)^2}{2\sigma^{+2}}-\frac{(\varepsilon_1^++\Delta\varepsilon-\mu_2^-)^2}{2\sigma^{-2}}]d\varepsilon_1^+, \end{aligned} \qquad (10)$$

$$\begin{aligned} p_{22}(\Delta\varepsilon)&=\int_{\mu_2^+-3\sigma^+}^{\mu_2^++3\sigma^+} g(\varepsilon_2^+)d\varepsilon_2^+\int_{\mu_2^--3\sigma^-}^{\mu_2^-+3\sigma^-} g(\varepsilon_2^-)\delta(\varepsilon_2^--\varepsilon_2^+-\Delta\varepsilon)d\varepsilon_2^-\\ &=\frac{\nu_{22}}{2\pi\sigma^-\sigma^+}\int_{\mu_2^+-3\sigma^+}^{\mu_2^++3\sigma^+}\exp[-\frac{(\varepsilon_2^+-\mu_2^+)^2}{2\sigma^{+2}}-\frac{(\varepsilon_2^++\Delta\varepsilon-\mu_2^-)^2}{2\sigma^{-2}}]d\varepsilon_2^+, \end{aligned} \qquad (11)$$

where $\nu_{11}=(1-\alpha^-)(1-\alpha^+)$, $\nu_{12}=(1-\alpha^-)\alpha^+$, $\nu_{21}=\alpha^-(1-\alpha^+)$, $\nu_{22}=\alpha^-\alpha^+$, and $\Delta\varepsilon \geq 0$ is the energy of absorbed hydrated electron.

Using $x=(\varepsilon^+_k-\mu^+_k)/\sigma^+$, $\beta=\sigma^+/\sigma^-$,

$y_{ik}=(\Delta\varepsilon-\Delta\mu_{ik})/\sigma^+$, $\Delta\mu_{ik}=\mu^-_i-\mu^+_k>0$, we can reduce (8) – (11) to the simple formula

$$\begin{aligned} p_{ik}(y_{ik})&=\frac{\nu_{ik}}{2\pi\sigma^-}\\ &\times\int_{-3}^{3}\exp[-\frac{x^2}{2}-\beta^2\frac{(x+y_{ik})^2}{2}]dx \end{aligned} \qquad (12)$$

Introducing $a=(1+\beta)^2/2$, $b_{ik}=y_{ik}\beta^2/2$, $c_{ik}=y_{ik}\beta^2/2$, one can write (12) in the form

$$\begin{aligned} p_{ik}(y_{ik})&=\frac{\nu_{ik}}{2\pi\sigma^-}\\ &\times\int_{-3}^{3}\exp[-(ax^2+2b_{ik}x+c_{ik})]dx \end{aligned} \qquad (13)$$

and to obtain the following result

$$\begin{aligned} p_{ik}(y_{ik})&=\frac{\nu_{ik}\beta}{4\sqrt{\pi a}}\exp(\frac{b_{ik}^2-ac_{ik}}{a})\\ &\times[\mathrm{erf}(3\sqrt{a}+\frac{b_{ik}}{\sqrt{a}})+\mathrm{erf}(3\sqrt{a}-\frac{b_{ik}}{\sqrt{a}})] \end{aligned} \qquad (14)$$

according to integral [20]

$$\begin{aligned} &\int\exp[-(ax^2+2bx+c)]dx=\frac{\sqrt{\pi/a}}{2}\exp[\frac{b^2-ac}{a}]\\ &\times\mathrm{erf}(\sqrt{a}x+\frac{b}{\sqrt{a}})+C \quad \text{where} \quad C=cons,\ a\neq 0\\ &\text{and}\ \ \mathrm{erf}(-x)=-\mathrm{erf}(x). \end{aligned}$$

Then, the absorption spectrum $P(\Delta\varepsilon)$ of hydrated electrons can be represented by formula

$$P(\Delta\varepsilon)=A$$

$$\times(p_{11}+p_{12}-p_{11}p_{12}+p_{21}+p_{22}-p_{21}p_{22}) \quad (15)$$

where $A$ is the constant of normalization for providing $P_{max}(\Delta\varepsilon)=1$ and the negative items are required for absorbed hydrated electrons to be included into the spectrum only once.

Introducing $y = y_{11} = (\Delta\varepsilon - \Delta\mu_{11})/\sigma^{+}$ ,

$d = (\delta^{-}+\delta^{+})/2\sigma^{+}$ , $y_{12} = y-(1+t)d$ ,

$y_{21} = y-(1-t)d$ , $y_{22} = y-2d$ , $\gamma = 1+\beta^{2}$ ,

$\delta^{-} = \sigma^{+}(1-t)d$ , $\delta^{+} = \sigma^{+}(1+t)d$ , $(-1<t<1)$,

$q = \sigma^{+}/k_{B}T$ , and

$$c = \frac{\sqrt{8\pi\gamma}}{\beta}[1+\exp(s^{-}-q(1-t)d)] \times[1+\exp(s^{+}-q(1+t)d)],$$

we will obtain the solution for specific "$i$" and "$k$" out of the formula (14):

$$p_{11}(y) = \frac{\exp(-\frac{\beta^{2}y^{2}}{2\gamma})}{c} \times[\mathrm{erf}(3\sqrt{\frac{\gamma}{2}}+\frac{\beta^{2}y}{\sqrt{2\gamma}})+\mathrm{erf}(3\sqrt{\frac{\gamma}{2}}-\frac{\beta^{2}y}{\sqrt{2\gamma}})] \quad (16)$$

$$p_{12}(y) = \frac{\exp(s^{+}-q(1+t)d-\frac{\beta^{2}y_{12}^{2}}{2\gamma})}{c} \times[\mathrm{erf}(3\sqrt{\frac{\gamma}{2}}+\frac{\beta^{2}y_{12}}{\sqrt{2\gamma}})+\mathrm{erf}(3\sqrt{\frac{\gamma}{2}}-\frac{\beta^{2}y_{12}}{\sqrt{2\gamma}})] \quad (17)$$

$$p_{21}(y) = \frac{\exp(s^{-}-q(1-t)d-\frac{\beta^{2}y_{21}^{2}}{2\gamma})}{c} \times[\mathrm{erf}(3\sqrt{\frac{\gamma}{2}}+\frac{\beta^{2}y_{21}}{\sqrt{2\gamma}})+\mathrm{erf}(3\sqrt{\frac{\gamma}{2}}-\frac{\beta^{2}y_{21}}{\sqrt{2\gamma}})] \quad (18)$$

$$p_{22}(y) = \frac{\exp(s^{-}+s^{+}-2qd-\frac{\beta^{2}y_{22}^{2}}{2\gamma})}{c} \times[\mathrm{erf}(3\sqrt{\frac{\gamma}{2}}+\frac{\beta^{2}y_{22}}{\sqrt{2\gamma}})+\mathrm{erf}(3\sqrt{\frac{\gamma}{2}}-\frac{\beta^{2}y_{22}}{\sqrt{2\gamma}})] \quad (19)$$

## The Results and Discussion

Using the equations (16) – (19) one can calculate the overall absorption distribution (15) for four hydrated-electrons transitions in dependence on the absorbed energy $\Delta\varepsilon$ and represent it in the graphic comparison with the experimental data at 274 K as shown in Figure 2 with the curve maximum at ~1.77 eV [1].

For this, we have used the calculation parameters given in the Table I where $\Delta\mu_{11}$ is the energy difference of two allowed local electron levels in the band gap of liquid water (see Figure 1a) when the first is the occupied-byelectron hydroxonium $H_3O$ and the second is the vacant hydroxyl OH. The dispersion $qk_B T$ $\sigma^{+}=qk_BT$ with $q$ = 0.33 by definition and $T$ = 274 K. The ratio $\beta = \sigma^{+}/\sigma^{-}$ in Table I is gotten from $P(\Delta\varepsilon_{exp} = 0.926) = 0.01$ and the parameter $d$ is defined by $2\sigma^{+}d = 1.83$ eV as the energy difference of the local electron levels of $(H_2O)^{-}_2$ and $(H_2O)^{+}_2$ minus 1.75 eV as shown in Figure 1b. The $t$, $s^{-}$ , and $s^{+}$ are adjustable parameters at the obvious condition $s^{+} > s^{-}$ due to $\sigma^{+} << \sigma^{-}$.

One can see in Figure 2 the satisfactory consent of the experimental data and the results of simulation by the model (15) – (19) of electron transitions between 4 energy levels in the band gap of water shown in Figure 1b [1].

It is important to underline that in this model, the excited states of hydrated electrons are the natural species of liquid water as $H_3O$ and $(H_2O)^{-}_2$ but not the quantum states of excited electron in the potential hollow sphere between water molecules.

In addition, the electron levels of $(H_2O)^{-}_2$ and $(H_2O)^{+}_2$ are appeared in the band gap of liquid water in the case of its photo-ionization or under the action of high dc voltage onto water as in the Lord Armstrong experiment [13]. It means that there are only two allowed electron levels in the band gap of pure water in the thermodynamic-equilibrium state and these levels are connected with the inherent species in liquid water $H_3O^{+}$ and $OH^{-}$.

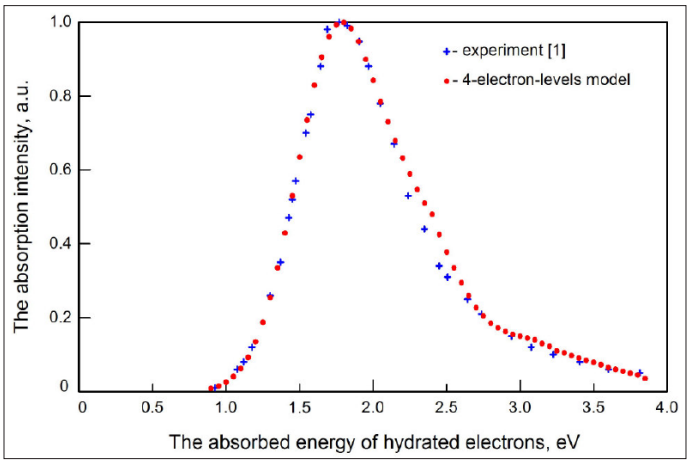


**Figure 2:** The absorption spectrum of hydrated electrons in bulk water at 274 K. The crisscrosses are the experimental data of hydrated electrons produced by electron beam in water; the red points are the simulation results in the 4-electron-levels model characterized by equations (15)–(19) with the convenient parameters out of Table I [1].

**Table I: The optimal calculation parameters for coincidence of the results of simulation by the equation (15) with the experimental data [1]**

| $\Delta\mu_{11}$, eV | $\sigma^{+}$, eV | $q$ | $\beta$ | $d$ | $t$ | $s-$ | $s+$ |
|---|---|---|---|---|---|---|---|
| 1.75 | 0.00779 | 0.33 | 0.028 | 117.5 | 0.38 | 23.25 | 51.48 |

## Conclusion

The hydroxide and hydroxonium ions $OH^{-}$ and $H_3O^{+}$ are the natural species of pure liquid water. They are associated respectively with the vacant electron level in the band gap and the occupied-by-electron one there. These levels lie symmetrically to the middle of the band gap which is Fermi's level $\varepsilon_F$ of the stoichiometric water. The energy difference between them is 1.75 eV as shown in Figure 1a. This energy difference forms the absorptionspectrum peak of hydrated electrons at the photo-ionization of pure water on 4 electron levels associated with non-equilibrium species: $(H_2O)^{-}_2$ , $H_3O$, OH, and $(H_2O)^{+}_2$ .

The simulation of absorption spectrum of hydrated electrons in bulk water at 274 K by the model of 4 electron transitions between

these species described by equations (15) – (19) gives very good consent with the experimental data [1]. This model attracts attention by assumption of the existence of excited hydrated electrons in the natural species of liquid water: $H_3O$ and $(H_2O)^-_2$ what gives a simple explanation of the experimental data.

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