

The Behavior of Water in Basic Sciences and its Applications after Hydrogen Bond Dissociation

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Abstract

It is said that water we use in daily life consists of several molecules connected with hydrogen bonding. However, the quantum dynamics of water after hydrogen-bond dissociation has not been researched so far, although there are many a study of water relating to bonding with its other chemical compounds. We focus on the hydrogen bond-dissociated water supposed to possess elementary particle-like matter after high pressure of approximately 100 MPa to water. The matter in the water is described as $\langle H^+ \sim e^- \rangle$, in which the proton and the electron exist neither separately nor forming hydrogen, and we call the quantum state the extended particle. Moreover, the particle exists for a long period stably. Here we wish to associate the macroscopic phenomena of water we usually encounter with the microscopic nature due to the function of the particle. The motivation of the research is essential to understand water from an idea of the particle. Furthermore, here, we wish to associate the usual macroscopic phenomena of water with the microscopic nature due to the function of the particle so that we can control to keep the water clean in an environment as another motivation. Furthermore, the reduction of radioactive cesium to change a stable barium atom was persuaded by taking into consideration the particle which enters into the radioactive substance. This is a breakthrough in the nuclear reaction without a huge energy outside. We discussed the mechanism of radiation reduction from a radioactive substance.

Finally, we investigate particle stability as a function of the distance between H^+ and e^- and focus on the overlap of their wave functions. The system is assumed to exist in a potential well that allows the stable existence of the particle from a theoretical viewpoint.

Introduction

Water is a universally found compound, and there are several reports on the behavior of water in the chemical, biological, and medical field. Therefore, we will not refer to the previous reports here, as they are already ample in number. There are also some basic textbooks, such as "The Nature of Chemical Bond" by L. Pauling [1], which include hydrogen bonding in water. And the hydrogen-bond kinetics in liquid water was discussed in the structure and diffusion process [2]. Besides, there are no reports that discuss the viewpoint from physics, although quantum mechanics was introduced [3] and there are computer simulation studies on the chemical structure of a water molecule in fullerene (C_{60}) chemical solution [4, 5]. There are also many studies on water molecules such as liquid [6], glassy [7], and the phase transition of water [8]. Furthermore, water research to other fields is discussed in biomolecules such as the cell membrane protein, aquaporin, through which only a single water molecule can pass, be it in plants or human body [9, 10]. A few unique technologies of water research are the dynamics of floating water bridges between two beakers under high voltage [11, 12]. There are other interesting studies in optical applications for water such as the quantum dissipative state of coherent water [13-15], which expresses the properties from an optical viewpoint; these represent the microscopic and macroscopic behaviors of water. However, all these studies dealt with relating to the electron(s). While many studies have been reported in the field of high-energy physics or engineering between the late 1990s and early 2000s. Some of them were conducted with palladium metal complexes and dry deuterium or hydrogen gas at 343 K (1 atm for about one to two weeks). After this, molybdenum and strontium in the ppm order

were obtained [16], and similar research studies were continued in the 2000s. In previous research related to the nuclear physics at the atmospheric condition with the pressurized water. The extended particle, infoton $\langle H^+ \sim e^- \rangle$, in the water [17] is formed after the dissociation of hydrogen bonds formed with two water molecules, which particle seems to be elementary particle-like. We name it SIGN water (Spin Information Gauge-field Network) after dissociated-hydrogen bond and we discussed along with the extended particles [18, 19] which is called infoton. Furthermore, the theoretical concept of spin and gauge relating to the infoton in the water has not been published yet. Our findings in the water result in many interesting behaviors of the infoton. We introduced some significant roles of the extended particles in the removal of pollutants from car exhausts [20] and in maintaining the freshness of foods [21]. Furthermore, here is another interesting theme associated with a nuclear disaster that occurred in Japan in March 2011. Since then, studies with the water have been performed to reduce the radioactivity from cesium-contaminated soils in Fukushima. We discovered stable barium from radioactive cesium (134 and 137) with weak energy (~ 0.03 eV) that infoton possesses by means of repeating the experiments from 2011 to 2013, leading to the equation for half-life reduction, which relates to nuclear transmutation [22, 23].

Thus, we have experimentally developed evidence of the function of SIGN water through the interaction between water and other substances due to the infoton. Here we mainly discuss the behavior of the water involving infoton with quantum mechanics how it exists stably, although remains to be experimentally observed.

Only introduction of the fabrication of the SIGN water here;

Water subjected to high pressures (100 MPa) results in the dissociation of hydrogen bonds. After that, the pico-sized water molecule might be indirectly evaluated with hydrogen-nuclear magnetic resonance spectroscopy (H-NMR) and Fourier-transform infrared (FTIR) spectroscopy [24], although this is not reported in the present paper. A theoretical approach using computer simulation of water by the molecular orbital method (DV- $X\alpha$, Discrete Variational $X\alpha$ potential) [25] revealed the status of an electron and/or the electromagnetic wave functions of the infoton, which possessed both particle and wave nature.

Quantum mechanical characteristics of extended particle, $\langle H^+ \sim e^- \rangle$; In terms of the wave function

The study considering hydrogen bonds refers to the abnormal behaviors in liquid water against its density [26]. In the same style, the relationship between structural order and the anomalies of liquid water was reported for quantitative understanding through the study of translational and orientational order [27]. However, more fine part must be essentially regarded rather than molecules with four neighbours and these structures which may generate with the results of the wave functions in each atom like oxygen and hydrogen.

It is presumed that the status of the extended particle, infoton $\langle H^+ \sim e^- \rangle$, was defined after the dissociation of the hydrogen bonds between two water molecules, as revealed by computer simulation using the DV- $X\alpha$ method. Microscopically, the infoton possesses both electromagnetic wave nature as well as particle nature, as the e^- in this species neither remains bound to the hydrogen atom nor does it separate from H^+ , i.e., there is no separate proton and electron. Owing to this nature, the particle can function in chemical reduction as well as transmutation in nuclear physics as shown previously. We have several evidences for the macroscopic behavior of water, which we have developed over several years, as described above. First, let us consider the stability of the extended particle, infoton $\langle H^+ \sim e^- \rangle$, as a function of the distance between the proton and electron.

The usual Schrödinger wave function is as follow;

$$\left\{ -\frac{1}{2}\nabla^2 + V(r) \right\} \chi(r) = E \chi(r) \text{ to } \chi(r) = R(r) Y(\theta, \varphi), \quad (1)$$

Where $Y(\theta, \varphi)$ is the spherical harmonics, which can be solved using the usual method wherein the potential $V_l(r)$ is a function of the distance and is given by the following equation in terms of the quantum numbers m and l :

$$V_l(\mathbf{r}) = V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \quad (2)$$

Distances of electron from proton; r_1 , r_2 , and r_3
Case 1 $\langle H^+ \sim e^- \rangle$, r_1 : electron is close to proton
Case 2 $\langle H^+ \sim \sim e^- \rangle$, r_2 : “infoton”
Case 3 $\langle H^+ \sim \sim \sim e^- \rangle$, r_3 : each proton and electron, just before ionization (neither proton nor electron)

Figure 1: Definition of the distance between electron and proton in the extended particle.

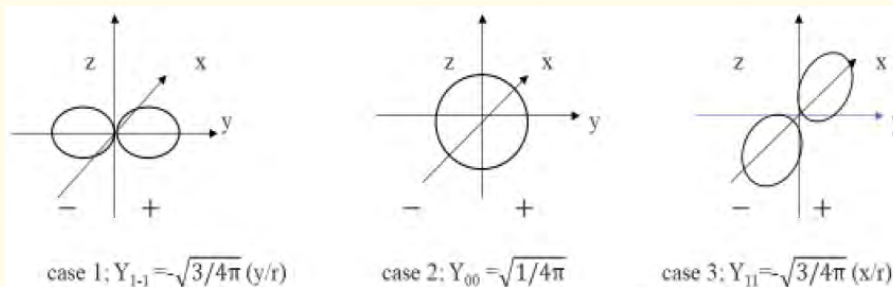


Figure 2: Real spherical harmonics corresponding to the distance between the proton and electron in infoton $\langle H^+ \sim e^- \rangle$.

The real spherical harmonics are given corresponding to the atomic orbitals shown in Fig. 2. A close inspection of the three cases shown in the figure suggests that the smallest distance between the proton and electron is r_1 (Case 1), and there is a negative charge around H^+ . The distance, r_2 , shown in Case 2, is the intermediate between Case 1 and Case 3 and resembles a positron around the little space where the electron moves apart, similar to a covalent bond. Finally, the largest distance, r_3 , can be seen in Case 3, which is composed of a positron, according to Dirac’s theory.

Momentum, p , is a convenient parameter in treating the potential when we consider the movement of infoton under a potential. In classical dynamics, the Hamiltonian is described as follows:

$$H(p, x) = \frac{1}{2m}(p \cdot p) + V(r) \tag{3}$$

The wave function is

$$\chi(r, t) = a \exp \left[-\frac{i}{\hbar} \{ (p \cdot r) - E t \} \right] \tag{4}$$

This function has a wave vector p/\hbar , which is described in terms of frequency, ν , as follows:

$$\nu = W/2\pi\hbar = 1/2m (p \cdot p) \tag{5}$$

The energy (joules) is calculated using the equation, $E = p^2/2m = (2\pi\hbar/L)^2/2m$, where L is the distance. The energy E of atomic hydrogen is calculated to be 4.3 eV using the size of the hydrogen atom (78 pm or 78×10^{-12} m), which is larger than that of the proton (66×10^{-15} m) [28].

Let us consider Case 1. This situation corresponds to the binding energy of the proton and electron forming the hydrogen atom, and it can be assumed to be 4.3 eV, in analogy with the H-H bond energy. In Case 3, the proton is almost separated from the electron and is on the verge of ionization, although it may not go very far. The corresponding energy can be assumed to be 13.5 eV, which is necessary

to draw an electron from the proton. Now, we need to determine the energy of the infoton $\langle H^+ \sim e^- \rangle$. Before that, it is worth estimating the distance between the proton and electron in all the cases; the covalent bond “c.30 Pm [28] in Case 1, and Case 3 can be regarded as the distance of the hydrogen atom as Van der Waals, 120 Pm [28]. This estimation seems reasonable according to the length of the hydrogen bond (189 Pm) [25]. Now, we can estimate the assumed distance (45 Pm) for the infoton $\langle H^+ \sim e^- \rangle$ from these values. In Case 1, $Y_{1,-1} = -\sqrt{3/4\pi} (y/r) = -1.467$ in Case 2, $Y_{00} = \sqrt{1/4\pi} = 0.282$; and in Case 3, $Y_{11} = -\sqrt{3/4\pi} (x/r) = -2.822$. These values are multiplied by the hydrogen-like radial function, $R_{10}(r) = Z^{3/2} \cdot 2e^{-Zr} / \sqrt{2}$, $\zeta = \frac{Z}{n}$, electrical charge; n, quantum number 1 in hydrogen atom. Then, $R_{10}(r) \cdot Y_{1,-1} = 0.391$ in Case 1, $R_{10}(r) \cdot Y_{00} = 0.564$ in Case 2, and $R_{10}(r) \cdot Y_{11} = 0.188$ in Case 3. Therefore, the status of the wave function is largest in Case 2, corresponding to the infoton.

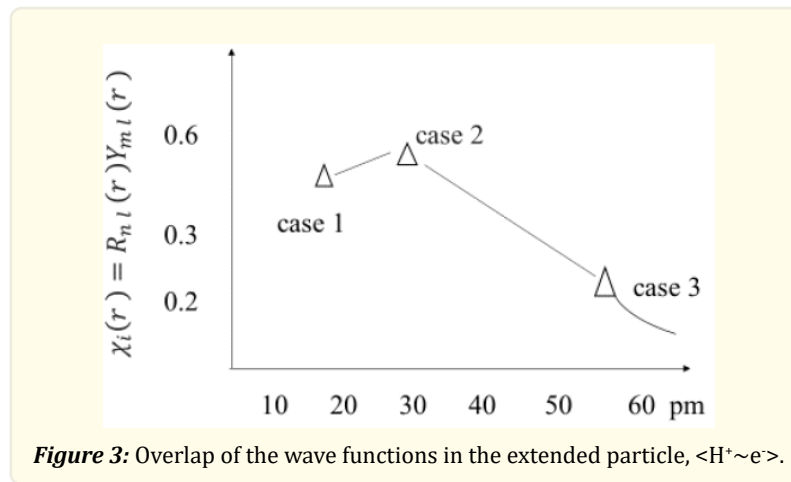


Figure 3: Overlap of the wave functions in the extended particle, $\langle H^+ \sim e^- \rangle$.

Potential of the extended particle

There are some discussion researches with quantum dimer associating with hydrogen bond in angle/distance potential energy [29]. They discussed energy and atomic charges as a function of hydrogen bond angle and O-O distance by computer simulation method and concluded that hydrogen bond angle appeared to play the largest part in determining H-bond strength with O-O distance. However, they did not discuss the causes to determine the O-O distance and not had any kind of experimental data, although analysis was performed in an atomic level. Regarding with potential energy, the surface of H---H₂O was computed in the region of van der Waals [30], which seems to be close to the potential energy corresponding to Fig. 4.

Another calculation for the stability of the infoton can be achieved using Eq. (2). The potential can then be obtained as follows: the second term in Eq. (2), $\frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}$, is calculated in terms of the quantum number l, which is equal to 1; r is the distance in Case 3 and can be regarded as half the distance (120 Pm) of the hydrogen atom, that is, 60 Pm (Figure 4), within which the particle can exist in a square potential well.

Another point of stability of the extended particle, infoton $\langle H^+ \sim e^- \rangle$

The importance of SIGN water in daily life is based on the stability of the infoton. The information of infoton refers to the momentum (defined with velocity and mass of infoton). Here is a research of ultrafast memory loss and energy redistribution in the hydrogen bond network of liquid H₂O [31], which can be deserved with the application of water.

The second point of stability is concerned with whether some of the water molecules could be coherent with the extended particles if they still exist after the dissociation of the hydrogen bonds. Various macroscopic pieces of evidence support such existence and stability of the particles, although these could not be observed under an electron microscope. Here is another interesting report which is

performed with TEY-NEXAFS (total electron yield near-edge x-ray absorption fine structure) on an observable rearrangement in liquid water based on the energetics of hydrogen bond and network [32]. Stability corresponds to their endurance without being attached to the original water molecules, even if some of them remained after conversion to smaller molecules. The infoton involving an electron and a proton could be understood from the viewpoint of elementary particle physics. Here, we consider that the particle is close to the potential barrier and collides with the wall (Fig. 5).

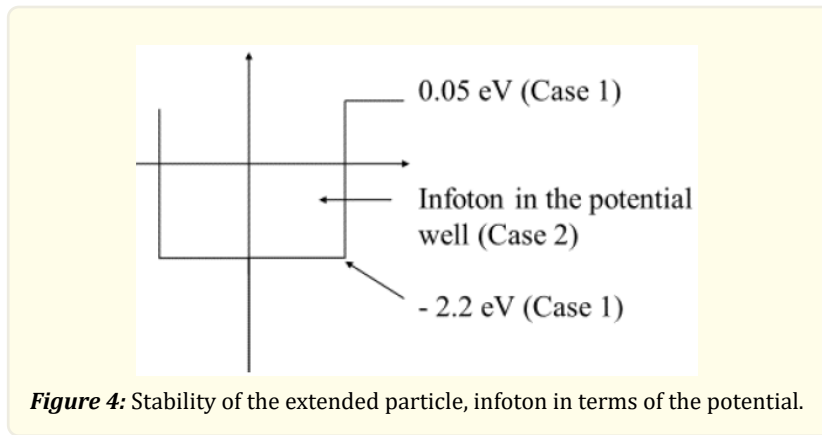


Figure 4: Stability of the extended particle, infoton in terms of the potential.

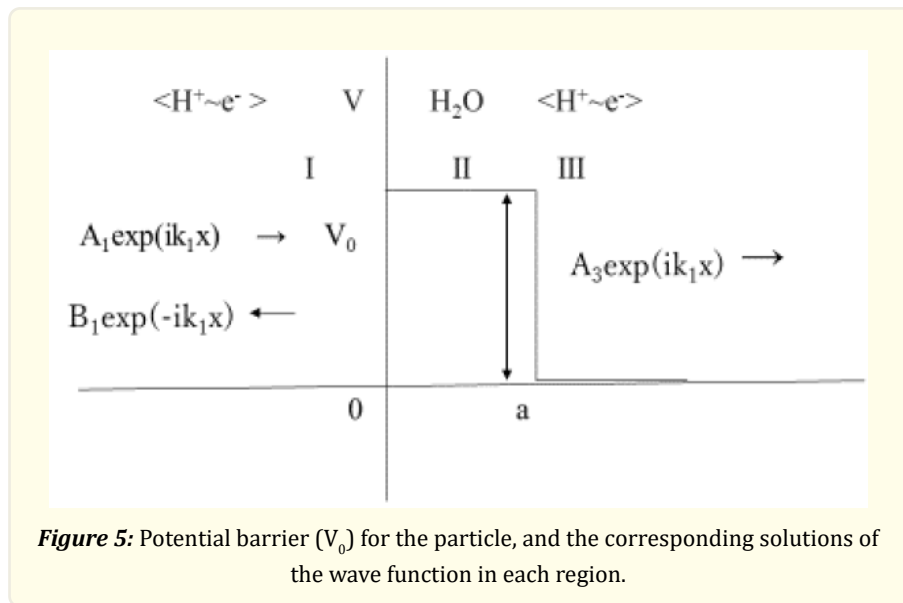


Figure 5: Potential barrier (V_0) for the particle, and the corresponding solutions of the wave function in each region.

Region I: Wave function

$$u_1 = A_1 \exp(ik_1 x) + B_1 \exp(-ik_1 x) \quad (6)$$

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \quad (7)$$

Now, we calculate the flow of possibility as follows:

$$S(x) = \frac{\hbar}{2im} \left[u_1^* \frac{du_1}{dx} - u_1 \frac{du_1^*}{dx} \right] = \frac{\hbar k_1}{m} (|A_1|^2 - |B_1|^2) \quad (8)$$

Here, $\frac{\hbar k_1}{m}$ is the velocity, v , of the particle (infoton) moving toward the right side, and $v|A_1|^2$ indicates the strength of the flow for

the wave function given in Eq. (6). The second term in Eq. (6) implies that the particle moving toward the left has strength of $v|B_1|^2$. Now, we develop the wave functions for regions II and III as follows:

Region II:

$$u_2 = A_2 \exp(ik_2 x) + B_2 \exp(-ik_2 x) \quad (9)$$

$$k_2 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} \quad (10)$$

Region III: Considering that there are no particles moving toward the left, the wave function can be represented as

$$u_3 = A_3 \exp(ik_1 x) \quad (11)$$

Since u and du/dx are continuous at $x = 0$ and $x = a$, we have

$$A_1 + B_1 = A_2 + B_2, \text{ at } x = 0 \quad (12-1)$$

$$k_1 (A_1 - B_1) = k_2 (A_2 - B_2) \quad (12-2)$$

$$A_2 \exp(ik_2 a) + B_2 \exp(-ik_2 a) = A_3 \exp(ik_1 a), \text{ at } x = a \quad (12-3)$$

$$k_2 (A_2 \exp(ik_2 a) - B_2 \exp(-ik_2 a)) = k_1 A_3 \exp(ik_1 a) \quad (12-4)$$

Eliminating A_2 and B_2 from Eq. (12-1) to (12-4), the ratios B_1/A_1 and A_3/A_1 are obtained.

Considering regions I and III, the strengths of the ratios $|B_1/A_1|^2$ and $|A_3/A_1|^2$ are the defined reflection and transparency, respectively, as B_2 is eliminated.

Moreover, as $E < V_0$, we can conclude the following:

$$k = \sqrt{\frac{2m(E-V_0)}{\hbar^2}} = i \kappa_2$$

$$\text{Reflection} = \left| \frac{B_1}{A_1} \right|^2 = \left[1 + \frac{4E(V_0 - E)}{V_0^2 \sinh^2 k a} \right]^{-1}$$

$$\text{Transparency} = \left| \frac{A_3}{A_1} \right|^2 = \left[1 + \frac{V_0^2 \sinh^2 k a}{4E(V_0 - E)} \right]^{-1} \quad (13)$$

In quantum theory, reflections will occur when $E > V_0$, and transparency will be obtained when $E < V_0$, which is called the tunnel effect. However, there will be no reflection at $k_2 a = \pi, 2\pi, \dots$.

Therefore, infoton $\langle H^+ \sim e^- \rangle$ can go through the potential in water, which provides transparency in the order of terahertz, although normal water should adsorb such longer wavelengths. We have already confirmed this by examining the longer wave regions using FTIR spectroscopy [24].

Conclusion

After dissociation of hydrogen bonds, the extended particles in water are presumed to possess $\langle H^+ \sim e^- \rangle$, which is neither an ion nor an atom; the two entities are neither bound nor separated with respect to each other. Then, we discussed the reason for the stability of the particle itself and why it does not reverse over a long period of time to form the original water molecule. Finally, we introduced the concept of stable existence of SIGN water. A variety of macroscopic evidence are experienced by many people who use water in daily life, resulting in the easier elucidation of these phenomena in the theory. In the future, we study how infoton transfers via a gauge field or electromagnetic field besides finding infoton.

Author contributions

Sunao Sugihara conceptualized and performed the study, and authored the manuscript.

Competing interest declaration

Competing interests Submission of a signed Competing Interests Statement is required for all content of the journal.

References

1. Pauling L. The Nature of Chemical Bond, 3rd edition, George Banta Company Inc (1960).
2. Luzar A and Chandler D. "Hydrogen-bond kinetics in liquid water". Letters to Nature 379 (1996): 55-57.
3. Coolidge AS. "A Quantum Mechanics Treatment of the Water Molecule". Phys. Rev 42 (1932): 189-209.
4. Kurotobi K and Murata Y. "A Single-Molecule of Water Encapsulated in Fullerene C₆₀". Science 333.6042 (2011): 613-616.
5. Huang X., et al. "New ab initio potential energy surface and the vibration-rotation-tunneling levels of (H₂O)₂ and (D₂O)₂". The J. of Chem. Phys 128.3 (2008): 034312.
6. Jorgensen W. "Revised TIPS for simulations of liquid water and aqueous solutions". J. Chem. Phys 77 (1982): 4156-4163.
7. Mishima O and Stanley HE. "The relationship between liquid, super cooled and glassy water". Nature 396 (1998): 329-335.
8. Millo A, Raichlen Y and Katzir A. "Mid-infrared Fiber-Optic Attenuated Total Reflection Spectroscopy of the Solid-Liquid Phase Transition of Water". Appl. Spectrosc 59 (2005): 460-466.
9. Yasui M., et al. "Rapid Gating and Anion Permeability of an Intracellular Aquaporin". Nature 402 (1999): 184-187.
10. Kozono D., et al. "Aquaporin Water Channels: Atomic Structure and Molecular Dynamics Meet Clinical Medicine". J. Clin. Invest 109.11 (2002): 1395-1399.
11. Fuchs EC., et al. "The Floating Water Bridge". J. Phys. D: Appl. Phys 40 (2007): 6112-6114.
12. Fuchs EC., et al. "A Floating Water Bridge Produces Water with Excess Charge". J. Phys. D: Appl. Phys 49 (2016): 1-7.
13. Tsenkova R. "Introduction Aquaphotomics: dynamic spectroscopy of aqueous and biological systems describes peculiarities of water". J. of Near-Infrared Spectrosc 17 (2009): 303-314.
14. Johansson B and Sukhotskaya S. "Allometric Scaling Behaviour—A Quantum Dissipative State Implies a Reduction in Thermal Infrared Emission and Fractal Ordering in Distilled Coherent Water". Water 3 (2012): 100-121.
15. Yokono T, Shimokawa S and Hattori H. "Infra-Red Spectroscopic Study of Structural Change of Liquid Water Induced by Sunlight Irradiation". Water 1 (2009): 29-34.
16. Iwamura Y., et al. "Elemental Analysis of Pd Complexes: Effects of D2 Gas Permeation". Jpn. J. Appl. Phys 41 (2002): 4642-4650.
17. Sugihara S. Infoton. Certificate of Trademark Registration by Japan Patent Office (No. 5138668) (2008).
18. Yukawa H. "Quantum Theory of Non-Local Fields, Free Fields, Part I". Phys. Rev 77 (1950): 219-226.
19. Yukawa H. "Quantum Theory of Non-Local Fields, Irreducible Fields and their Interaction, Part II". Phys. Rev 80 (1950): 1047-1052.
20. Sugihara S and Hatanaka K. "Photochemical Removal of Pollutants from Air or Automobile Exhaust by Minimal Catalyst Water". Water 1 (2009): 92-99.
21. Sugihara S, Suzuki C and Hatanaka K. "The Mechanism of Activation of Substances by Minimal Catalyst Water and Application in Keeping Foods Fresh". Water 3 (2011): 87-94.
22. Sugihara S. "Deactivation of Radiation from Radioactive Materials Contaminated in a Nuclear Power Plant Accident". Water 5 (2013): 69-85.
23. Sugihara S. "Faster Disintegration of Radioactive Substances Using The energy of Specially-Processed Water and Theoretical Prediction of Half-Life of Radionuclide". Int. J. Current Research and Academic Rev 3 (2015): 196-207.
24. Sugihara SK, Utsunomiya U and Yamaguchi S. Certificate of Patent No. 6666528. Japan Patent Office (2020).
25. Adachi H. Introduction of Quantum Materials Chemistry---Approach from DV-X α method--- (Sankyo Shuppan, Tokyo) (1993): 161-164.
26. Errington JR and Debenedetti PG. "Relationship between structural order and the anomalies of liquid water". Nature 409 (2001): 318-321.
27. Sastry S. "Order and Oddities". Nature 409 (2001): 300-301.

28. Emsley J. The Elements, the 3rd edition, Clarendon Press, Oxford (1998).
29. Scott JN and Vanderkooi JM. "A New Hydrogen Bond Angle/Distance Potential Energy Surface of the Quantum Water Dimer". *Water* 2 (2010): 14-28.
30. Zhang Q, Sabelli N and Bush V. "Potential energy surface of H—H₂O". *J. Chem. Phys* 95 (1991): 1080-1085.
31. Cowan ML, et al. "Ultrafast memory loss, and energy redistribution in the hydrogen bond network of liquid H₂O". *Nature* 434 (2005): 199-202.
32. Smith JD, et al. "Energetics of Hydrogen Bond Network Rearrangements in Liquid Water". *Science* 306 (2004): 851-853.

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