

Considering the Temperature Dependence of the Effective Density of States when Calculating the Band Gap Using the Values of the Ionic Product of Water

Stanislav V. Yefimov^{1*}

¹Analytical Lab, 2138 Orange Dr, Holiday, FL 34691

DOI: <https://doi.org/10.36347/sjpm.2026.v13i03.001>

| Received: 19.01.2026 | Accepted: 24.02.2026 | Published: 03.03.2026

*Corresponding author: Stanislav V. Yefimov
 2138 Orange Dr, Holiday, FL 34691

Abstract

Original Research Article

The study determined the band gap of water with higher accuracy by considering the temperature dependence of constant. The obtained value is among the band gaps of known semiconductors. The hypothesis that water and ice are semiconductors was confirmed.

Keyword: Water, electrolyte, semiconductor, band gap.

Copyright © 2026 The Author(s): This is an open-access article distributed under the terms of the Creative Commons Attribution 4.0 International License (CC BY-NC 4.0) which permits unrestricted use, distribution, and reproduction in any medium for non-commercial use provided the original author and source are credited.

INTRODUCTION

A chain of consistent studies led us to the need to determine band gap of water (Yefimov, S. 2025). The identity of the mathematical models of electrolyte solutions and doped semiconductors, which was shown in our previous works (Yefimov, S. 2023), (Yefimov, S. 2023), (Yefimov, S. 2024), (Yefimov, S. 2024), indicates the direction of the search for semiconductor properties of water. Such a property has been discovered and claimed to be an invention called: "Diode made of ice" (Yefimov, S. 2025). In this invention, the analogue of a crystalline semiconductor doped with an n-type impurity is ice doped with an acid, and the analogue of a semiconductor doped with a p-type impurity is ice doped with a base. The experimental data obtained and their interpretation allowed us to draw a conclusion about the mechanism of ionization of electrolytes in water (Yefimov, S. 2025). The proposed mechanism complements and expands the Arrhenius hypothesis of electrolytic dissociation (Arrhenius, S. 1903). In this work, we used an improved method for determining the band gap of water. The resulting value ranks among the band gaps of known semiconductors.

MATERIALS AND METHODS

The calculation of the band gap (Electrons and Holes in Semiconductors. 2009) water was carried out using reference data on the dependence of the ionic product of water (Kw) on temperature (Haynes, W.

2014). The data was processed in a Microsoft Excel spreadsheet. Using reference data, the $pKw+3lg(T)$ dependence on the reciprocal absolute temperature ($1/T$) was plotted. Using the Least Squares Method, the experimental points were approximated by a straight line. The band gap (E_g) was extracted from the slope of the line.

RESULTS AND DISCUSSION

The Theory of Electrolytic Ionization considers water as a semiconductor, which means that the expression for the product of charge carrier concentrations in semiconductors (Yefimov, S. 2025) is applicable to it, and this product is the ionic product of water ($Kw = n_e \times n_h$). The Ionic product values of water have been measured at various temperatures and are included in reference books. Using this reference data, one can estimate the band gap of water using the well-known equation:

$$Kw = C \times e^{\frac{-E_g}{k \times T}} \quad (1),$$

where C- constant, $k=1.38E-23$ (J/K)- Boltzmann constant, E_g - the energy band gap, T- absolute temperature, n_e and n_h - the molar concentration of mobile charge carriers, negative (n_e) and positive (n_h) (Electrons and Holes in Semiconductors. 2009). Taking the logarithm of the expression (1), we obtain the value of pKw .

$$pKw = C + \left(\frac{E_g \times lg(e)}{k} \right) \times \frac{1}{T} \quad (2)$$

The $pK_w - 1/T$ dependence graph is approximated by a straight line, and the band gap is found from the slope of the line. Thus, we determined the band gap of water to be 0.53eV (Yefimov, S. 2025). For a more accurate estimate of E_g , it is necessary to consider that the constant "C" in equation (1) is the product of the effective densities of state of the valence band (N_v) and the conduction band (N_c):

$$N_c = 2 \times \left(\frac{m_e \times k \times T}{2 \times \pi \times \hbar^2} \right)^{3/2}, \quad N_v = 2 \times \left(\frac{m_h \times k \times T}{2 \times \pi \times \hbar^2} \right)^{3/2}, \quad N_c \times N_v = C \times T^3,$$

where C is a temperature-independent constant. Taking the latter into account, we transform formula (2):

$$pK_w + 3 \times \lg(T) = C + \left(\frac{E_g \times \lg(e)}{k} \right) \times \frac{1}{T} \quad (3)$$

Using reference data (Haynes, W. 2014), we plot the dependence of $pK_w + 3 \lg(T)$ on $1/T$ (Fig. 1). The experimental points are approximated by a straight line (Fig. 1, dotted line) using the least squares method. As a result, we obtain the slope and the intercept with the ordinate axis.

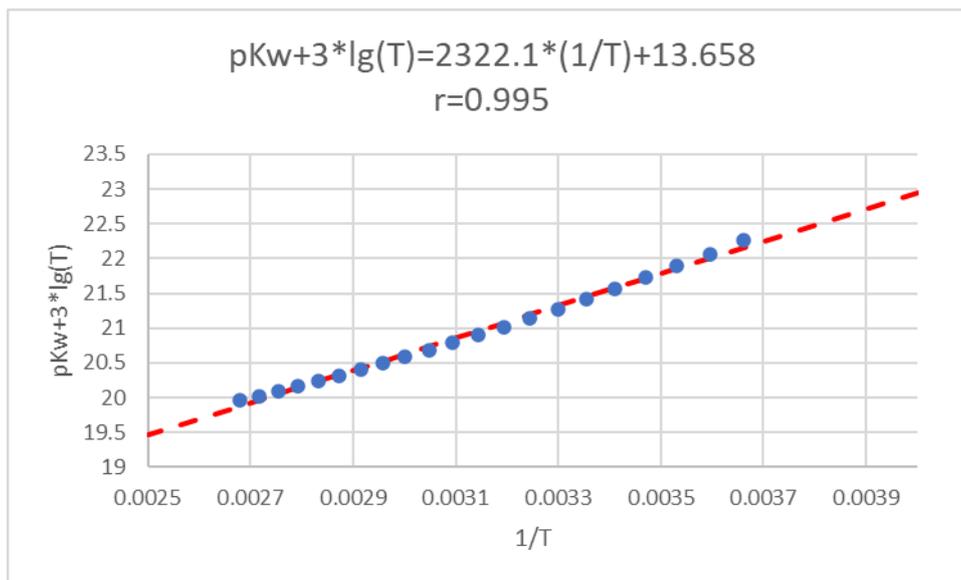


Figure 1: Dependence of $pK_w + 3 \lg(T)$ on $1/T$. Circles – reference data (Haynes, W. (2014)), dotted line – linear regression

Having performed simple calculations, we obtained $E_g = 0.46\text{eV}$. To check the correctness of the calculations, we substituted the obtained E_g , constant, and temperature $T = 298.15\text{K}$ into equation (3) and obtained the expected result: $pK_w = 14.0226$, and $K_w = 0.949\text{E-}14$. 0.46eV is less than calculated without the temperature correction (formula (2)), but the water position among semiconductors does not change, it is located between Indium antimonide ($E_g = 0.18\text{eV}$) and Germanium ($E_g = 0.67\text{eV}$). Available literature data, primarily calculated, on the band gap of water vary widely, from 5 to 14eV (Bischoff, T. *et al.*, 2021), (Fang, C. *et al.*, 2015). Such values are characteristic of true insulators and exclude the semiconducting properties of aqueous solutions. However, these semiconducting properties have been discovered and published not only by us but also by other researchers (Koncz, V. 2021), (Iván, I. *et al.*, 2005), (Hegedus, L. *et al.*, 1999). This contradiction will have to be resolved in the future. It should be noted that the authors of the latter studies, unlike us, attempt to explain the observed effects within the framework of the Arrhenius hypothesis. **The Law of electrolytic ionization:** “Water is a semiconductor. In water, acids ionize by donating an electron to the conduction band, while bases ionize by accepting an electron from the hole conduction band, forming a hole. Salt solutions are the

product of the interaction of an ionized acid and an ionized base”.

CONCLUSION

The more precise determined band gap of water (0.46eV) is a good confirmation of the law of electrolytic ionization. Among semiconductors, water occupies a position between Indium antimonide ($E_g = 0.18\text{eV}$) and Germanium ($E_g = 0.67\text{eV}$). The law of electrolytic ionization does not replace the Arrhenius dissociation model but rather complements and expands the methods for describing the behavior of electrolyte solutions.

REFERENCES

- Yefimov, S. (2025) Determination of the Band Gap of Water. Sch J Phys Math Stat, 12(9): 432-434. <https://saspublishers.com/article/23359/download/>
- Yefimov, S. (2023). General equation of state of acid-base balance in solutions. Resolution of the equation with respect to hydrogen ion concentrations and concerning the amount of added base or acid. Titration curves. Sch Acad J Biosci, 11(3), 122-129. <https://saspublishers.com/article/14111/>

- Yefimov, S. (2023). Finding Singular Points of the Titration Curve by Solving the Equation of State of the Electrolyte Solution. Sch Acad J Pharm, 12(3), 74-78.
https://www.saspublisher.com/media/articles/SAJP_123_74-78_FT.pdf.
- Yefimov, S. (2024). Derivation of the General Equation of State for a Doped Semiconductor. The Equation is Solved Concerning the Election Concentration in the Conduction Band for Different Concentrations and Properties of Doping Substances. Sch. J Eng Tech, 12(11), 324-331.
<https://saspublishers.com/article/20947/download/>.
- Yefimov, S. (2024). Finding singular points of the concentration curve of doped semiconductors. Sch. J Eng Tech, 12(12), 374-379.
<https://saspublishers.com/article/21194/download/>.
- Yefimov, S. (2025). Diode Made of Ice. Sch J Eng Tech, 13(1), 1-5.
<https://www.saspublishers.com/article/21365/>.
- Yefimov, S. (2025). Theory of Electrolytic Ionization. Sch J Eng Tech, 13(6), 377-380.
<https://doi.org/10.36347/sjet.2025.v13i06.002>.
- Arrhenius, S. (1903). Development of the theory of electrolytic dissociation, Svante Arrhenius - Nobel Lecture (accessed: 10/29/2025).
- Electrons and Holes in Semiconductors. (2009).
https://www.chu.berkeley.edu/wp-content/uploads/2020/01/Chenming-Hu_ch1-3.pdf (accessed: 10/29/2025).
- Haynes, W. (2014) Handbook of chemistry and physics 95 edition, CRC Press.
- Bischoff, T., Reshetnyak, I., Pasquarello, A. (2021) Band gaps of liquid water and hexagonal ice through advanced electronic-structure calculations. PHYSICAL REVIEW RESEARCH 3, 023182, 1-19.
<https://link.aps.org/pdf/10.1103/PhysRevResearch.3.023182>
- Fang, C., Li, W., Koster, R., Klimes, J., Blaaderena, A., Huis, M. (2015) The accurate calculation of the band gap of liquid water by means of GW corrections applied to plane-wave density functional theory molecular dynamics simulations Phys. Chem. Chem. Phys., 17, 365-375.
https://web.science.uu.nl/scm/Articles/2015/Fang_PhysChemChemPhys_2015.pdf
- Koncz, V. (2021) Modeling of acid-base diodes. Budapest University of Technology and Economics, 14 p.
<https://repozitorium.omikk.bme.hu/bitstreams/11d39b1c-15a0-406f-9a67-9adb833520eb/download>
- Iván, I., Simon, P., Wittmann, M., Noszticzius, Z. (2005) Electrolyte diodes with weak acids and bases. I. Theory and an approximate analytical solution. J Chem Phys 22;123(16):164509. DOI: 10.1063/1.2085047
- Hegedus, L., Kirschner, N., Wittmann, M., Simon, P., Noszticzius, Z., Amemiya, T., Ohmori, T., Yamaguchi, T. (1999) Nonlinear effects of electrolyte diodes and transistors in a polymer gel medium. Chaos. 9(2):283-297. DOI: 10.1063/1.166405.