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UDC 519.004.942
DOI: 10.20535/SRIT.2308-8893.2024.4.04

QUANTUM MECHANICS APPROXIMATION APPROACH TO INVESTIGATE MOLECULAR BEHAVIOR IN NITROGEN BINDING TO ENZYMES AND PROTEINS: IMPLICATIONS FOR BIOFUEL PRODUCTION

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Abstract. This research delves into the essential mechanisms underlying the binding of Nitrogen (N) atoms to enzyme molecules and their implications for protein formation in food crops and biogas production. Nitrogen (N), along with Phosphorus (P) and Potassium (K), plays a pivotal role in soil fertility and crop growth. The study explores the interactions between atoms through various mechanisms, such as catalysts, photosynthesis, and adiabatic reactions, to comprehend their roles in facilitating organic molecule formation. Additionally, the research examines the influence of enzymes on amino acids and their contributions to protein structure. The simulation process employs the Hamiltonian equation to quantify energy intensities and explore the effectiveness of adiabatic reactions in organic transformations. By investigating the molecular interactions in enzyme-catalyzed processes, this research aims to enhance protein formation in crops and optimize biogas production.

Keywords: nitrogen binding, enzyme molecules, protein formation, adiabatic reactions, biogas production, organic molecule formation.

INTRODUCTION AND BACKGROUND

Phosphorus (P), Potassium (K), and Nitrogen (N) are key elements in soil for growing food crops. Besides the other nutrients like calcium, magnesium, and sulfur, they form the foundation of soil and crop cultivation. Among them, Nitrogen is a fundamental building block for amino acids, proteins, and chlorophyll, which are necessary for plant growth and photosynthesis, and it is a key component of DNA, RNA, and other essential plant molecules [1].

Many organic reactions require an input of energy to overcome activation barriers and facilitate the conversion of inorganic molecules into organic compounds. This energy can be provided through various ways, including heating, irradiation with light, or the presence of catalysts.

Proton capture is an adiabatic reaction where a proton (H^+) is incorporated into a molecule, leading to the formation of a new compound. In the process of organic molecule formation, proton capture can occur when inorganic molecules react with protons to form organic molecules. While proton capture can contribute to the adiabatic process of organic molecule formation, it is just one of several mechanisms in the formation of organic molecule formation from inorganic precursors such as Nitrogen in inorganic form [2].

The specifics of the reactions involved in proton capture processes can vary depending on the particular inorganic molecules and the conditions under which they occur. Additionally, other factors such as the presence of catalysts or energy sources can influence the efficiency and outcomes of proton capture. It is noted that organic molecule formation is a complex and diverse field of study, and the processes involved can be influenced by numerous factors.

Photosynthesis contributes to proton capture in amino acids indirectly by producing NADPH (nicotinamide adenine dinucleotide phosphate oxidase) during the light-dependent reactions. The NADPH, in turn, supplies the necessary reducing power for the Calvin cycle, where carbon dioxide is converted into carbohydrates, including the building block for amino acid synthesis [3].

Enzymes influence proton capture in target amino acids as catalysts. Enzymes influence the formation of protein structure, but not by consuming itself. The interaction happens through their electrostatic field made by the electrostatic potentials of the atoms held by the enzyme and the targeted amino acids of the protein [4].

Fermentation process in biogas production from wheat and maize involves a series of physical reactions facilitated by various groups of microorganisms, leading to the generation of biogas, which is primarily composed of methane (CH_4) and carbon dioxide (CO_2) [5]. In the fermentation process of wheat/maize, the primary microorganism involved is yeast, and the key enzyme responsible for the conversion of sugars into ethanol (alcohol) and carbon dioxide is called "zymase". The typical atoms included in this enzyme are as same as in the other enzymes' atoms shown in Table 1 [6].

The formation of organic molecules from inorganic molecules can occur through various processes, including biological and non-biological pathways. While it is possible some organic reactions to occur at room temperature or under normal conditions without external heating, the generalization that all organic reactions can proceed adiabatically (without heat exchange with the surroundings) or at ambient temperature is not accurate. With this research, we will estimate the degree of the contribution to the organic molecule formation by adiabatic process and by other processes.

RESEARCH OBJECTIVES

The primary goal of this research is to investigate the fundamental mechanism of binding a Nitrogen atom to an enzyme molecule. The study aims to enhance protein formation in food crops and biogas production, focusing on Nitrogen in soil, wheat, and maize crops, and the enzymes involved in their production, namely Glutamate and Nitrate Reductase. Additionally, the research will explore the composition of biogas production during this process, primarily consisting of methane and carbon dioxide.

The main simulated physical reactions include:

1. Adiabatic Perturbation: This aims to understand the interactions between protons and targeted atoms of the amino acids, which play a crucial role in the binding process.
2. Electrostatic Perturbation: This analysis focuses on the influence of enzymes in accelerating the formation of proteins in specific targeted amino acids.

3. Photon Absorption and Electron Discharge: This part examines how photon absorption leads to electron discharge from the target atom.

To quantify the energy intensities of these physical reactions in the protein formation process involving the selected objects, the Hamiltonian equation will be utilized.

Furthermore, this research explores the effectiveness of adiabatic reactions in organic transformations. Specifically, it investigates whether certain organic reactions can occur at room temperature or under normal conditions without external heating, as this aspect is not yet clearly proven. The approximation method in quantum mechanics will be employed to assess the possibility of adiabatic reactions in comparison with photo synthesis and electrostatic energy fields produced by the catalyst (enzyme) in this context.

In conclusion, this research aims to provide essential insights into the binding of Nitrogen to enzyme molecules, which can contribute to improved protein formation in food crops and enhance biogas production.

METHODOLOGY

Selecting typical atoms in plant tissues and enzymes. A simplified system is considered, including typical atoms observed in wheat and maize as well as the atoms in enzymes in these crops, as shown in Table 1.

Calculating the probability of the reactions. Each of the adiabatic perturbation, electrostatic interaction, and the photon absorption, is calculated on each atom listed in Table 1. The algorithm of the calculation is shown in the latter section.

Table 1. Typical atoms observed in wheat and maize tissues

N	Typical atoms in tissue of the crops	Typical atoms in enzymes	Atomic number (Number of electrons)	Mass number	Empirically measured radius (re) in pico-meters [8]	Calculated diameter in pico-meters
1	Carbon (C)	Carbon (C)	6	12	70	140
2	Hydrogen (H)	Hydrogen (H)	1	1	25	50
3	Oxygen (O)	Oxygen (O)	8	16	60	120
4	Nitrogen (N)	Nitrogen (N)	7	14	65	130
5	Phosphorus (P)	Phosphorus (P)	15	31*	100	200
6	Potassium (K)	–	19	39*	220	440
7	Calcium (Ca)	–	20	40*	180	360
8	Magnesium (Mg)	–	12	24*	160	320
9	Sulfur (S)	Sulfur (S)	16	32*	100	200

* (the most common isotope, but there are others)

Comparing the result of the atomic level calculation with the molecular structure. Discussion will be made on the consistency of the calculated result with the actual molecular structure of glutamate synthetase (GS), which is essential for nitrogen uptake and assimilation from the soil. It helps convert inorganic nitrogen compounds, such as ammonium (NH_4^+) and nitrate (NO_3^-), into organic nitrogen forms like glutamate, with the following reaction [7]:

Glutamate + NH_4^+ + ATP → Glutamine + Pi.

Here, glutamate is an amino acid and serves as the precursor for glutamine synthesis. By incorporating ammonia, wheat utilizes GS to convert inorganic nitrogen (ammonium) into the organic nitrogen compound glutamine. "Pi" is an abbreviation for "inorganic phosphate". It refers to a form of phosphorus, an essential element for life, which exists in the inorganic state in chemical compounds.

Molecular form of Glutamate. The molecular formula of glutamate is $C_5H_9NO_4$. It is an organic compound composed of carbon (C), hydrogen (N), and Oxygen (O) atoms.

ALGORITHM (HAMILTONIAN EQUATION)

Hamiltonian equation consists of 6 terms: The kinetic energy of the target proton of amino acid, the potential of elastic electron scattering, the potential of electron capture, the electrostatic energy of catalyst (enzyme) to influence the targeted amino acid, and the photon absorption to drop an electron from the target amino acid. The first term, the kinetic energy of the target proton, is set as unity, which enables calculating relative probabilities of the occurrences of those terms.

Capture of an electron by a proton (charge exchange) in adiabatic process. The algorithm to calculate the probability of electron capture was taken from [9]. A case was considered, in which a proton of an atom, for example Oxygen, captured an electron of another atom, for example Hydrogen, which passed by the proton of the atom. Fig. 1 shows the coordinates of two protons and an electron. Two protons are symmetrically located on both sides of the origin O of the coordinate. $(1/2)R$ and $-(1/2)R$ are the coordinates (geometric positions) of two protons that will capture the electron of another atom. R is the distance between two protons, and the positions of these protons are fixed. On the other hand, r is the position of electron in a plane polar coordinate system and it changes as a function of geometric coordinate x, where $-(1/2)R \le x \le (1/2)R$.

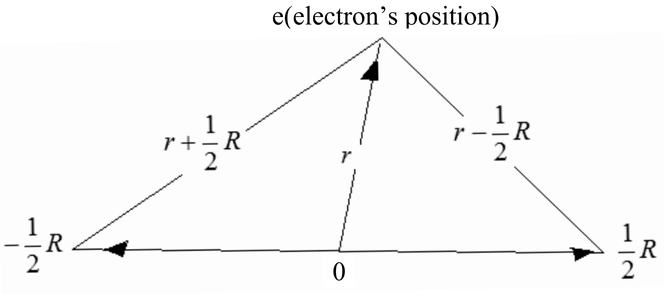


Fig. 1. The coordinates of the proton and the electron (adapted from [9] p. 89, Fig. 21)

Then it is assumed that the electron is initially attached to the proton at the coordinate of $(1/2)R$; then the initial state of the electron had the form, $\varphi = (r-(1/2)R)\cos wx$, where $\cos wx$ is the Eigen-wave function, w is the frequency of the oscillation of the electron, representing its energy level. Then, the probability of electron capture is calculated by the Hamiltonian equation shown below:

$$H = T_e - C_1\left(\frac{1}{r+(1/2)R}\right)\cos wx - C_2\left(\frac{1}{r-(1/2)R}\right)\cos wx\,, \tag{1}$$

where T_e is the kinetic energy of the electron. Here, it was assumed that the relative speed of proton was much slower than the electron's speed. Therefore, the geometry of an electron and protons was the main focus, not time dependency of the system. And, T_e was set as a unity (one).

When the electron is attached to one proton at the coordinate of $+(1/2)R$ as its initial state, the wave function is $(r-(1/2)R)\cos wx$; but, it changes to

$(r+(1/2)R)\cos wx$, when the electron is transferred to another proton located at $-(1/2)R$, as the process of the charge exchange.

The influence of enzyme to the amino acid by the electrostatic energy [10; 11] is described by the following equation:

$$E_{elec}=\sum_{i,j}\frac{q_i\,q_j}{4\pi\pi_0\cdot r_{ij}}\approx\frac{q_i\,q_j}{r_{ij}},$$

where E_{elec} is the electrostatic energy; q_i and q_j are the charges of the atoms; r_{ij} is the distance between the charges; and ε_0 is the vacuum permittivity.

The interaction with photon (from the interaction of a particle with the electromagnetic field, p. 45, [9]). Under the influence of the electromagnetic field, the momentum of a particle, p, becomes $p-eA/c$, where e is an electron charge, A is a vector potential of the electromagnetic field. Therefore the term of the Hamiltonian becomes:

$$\frac{p^2}{2m}-\frac{e}{mc}pA+\frac{e^2A^2}{2mc^2}.$$

The first term, $p^2/2m$, is T_e of (1). The second term is described by only angular coordinates, therefore we replace this term with an oscillation function $\cos\varphi$, where the frequency of φ is set higher than wx in order to simulate the light (photon). The third term is negligibly small.

By including the terms of kinetic energy, the elastic scattering, the electron capture, the electrostatic energy of the enzyme, and the photon absorption effect, the Hamiltonian becomes as the follow:

$$H=T_e-C_1\left(\frac{1}{r+(1/2)R}\right)\cos wx-C_2\left(\frac{1}{r-(1/2)R}\right)\cos wx-$$

$$-C_3\frac{1}{r_{i,j}}\cos wx-C_4\cos\varphi\cos wx\,.$$

When the reference [9] was published in 1969, a personal computers was not available, therefore the reference [9] further described the algorithm in mathematical forms with calculus, and predicted that the squared module of the coefficients, C_1, C_2, C_3 and C_4, gave the probability of charge exchange (the electron capture). However, in this research a personal computer was used to calculated the coefficients, C_1, C_2, C_3 and C_4 with the following algorithm of matrix algebra:

$$H=T_e-X\;\;c\,,$$

where X is made of four vectors, $-\left(\frac{1}{r+(1/2)R}\right)\cos wx$, $-\left(\frac{1}{r-(1/2)R}\right)\cos wx$, $1/(r_{ij})\cos wx$, $\cos\varphi\cdot\cos wx$. And c is the four column vector:

$$c=\begin{bmatrix}C_1\\C_2\\C_3\\C_4\end{bmatrix}.$$

Then a constraint was set

$$X'H = 0\,,$$

so

$$X'(T_e - Xc) = 0\,,$$

where X' is transpose matrix of X. Then,

$$X'Xc = X'T_e\,,\quad c = (X'X)^{-1}X'T_e\,.$$

SIMULATION PROCESS

For this simulation the values of R were assigned as the diameters of Hydrogen, Carbon, Nitrogen, Oxygen, Phosphorus, Potassium, Calcium, Magnesium, and Sulfur, as shown in Table 1, and r is given by (11), where x is the distance from the origin O toward $(-(1/2)R)$ and toward $(+(1/2)R)$ in Fig. 1, while the origin O is located at $x = 13$: and $(-(1/2)R)$ is at $x = 1$, and $(1/2)R$ is at $x = 25$.

Note: According to [9], p. 84, "Capture of an Electron by a Proton (Charge Exchange)" of the Chap. 2.4 "Adiabatic Perturbations", R is the distance between the two protons of Fig. 1. Here an assumption was made as if two same atoms, which were centered by each of two protons, were located next to each other: therefore, $R = 2 \times r$, where r is empirically measured radius of Table 1.

In our simulation for the adiabatic process, a symmetric geometry of two atoms was assumed as the mirror images on the both-sides of the origin O, as shown in Fig. 2. We assign the value of R by the empirically measured radius, 25 pico-meters, for example of hydrogen-atom [10]. Because two hydrogen-atoms are placed next to each other in Fig. 2, we assign 50 to the value of R. If charge exchange happens, the electron's plane polar coordinate, r, changes its position from the initial position, $+R/2$ of x-coordinates, to the position of the charge exchange, $-(1/2)R$. Then the relation between r and R is:

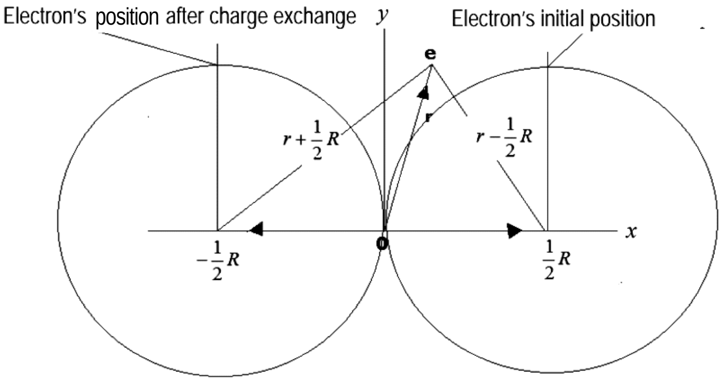


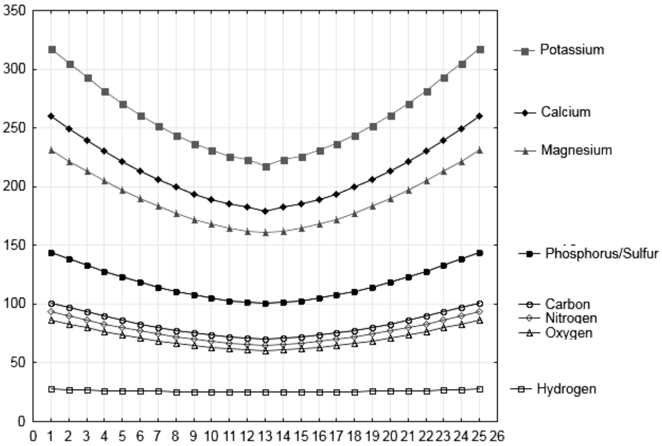
Fig.2. Position of the electron and its coordinate r

$$r = \sqrt{\left(\frac{R}{2}\right) + x^2}\,, \tag{2}$$

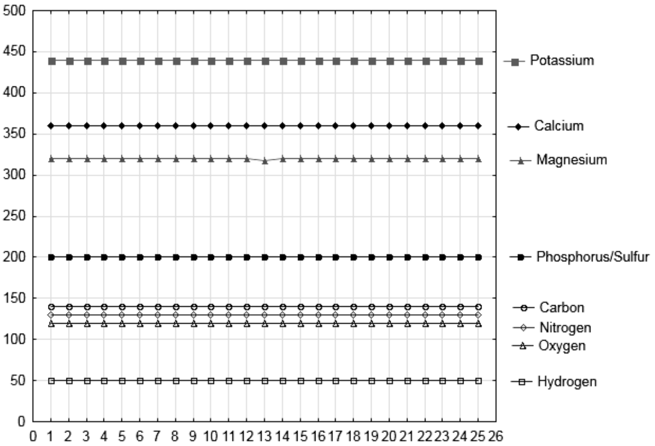
where x is the distance from the origin O toward $-(1/2)R$ and toward $+(1/2)R$, and the origin O is at 0 on the x-axis, $-(1/2)R$ is at –12 on the x-axis; and, $+(1/2)R$ is at +12 on the x-axis. The electron is initially attached to the proton at $+(1/2)R$ of x-coordinates; and then it will be attached to the proton at $-(1/2)R$ of x-coordinates after the charge exchange.

When the nucleons are far apart, the electron will be localized near one or the other proton. However, it doesn't mean that R in this simulation should be far apart to infinity, but it only justifies the wave functions of hydrogen-atom that distinguish the initial state of the wave function $(r-(1/2)R)\cos wx$ and the wave function $(r+(1/2)R)\cos wx$ after the charge exchange.

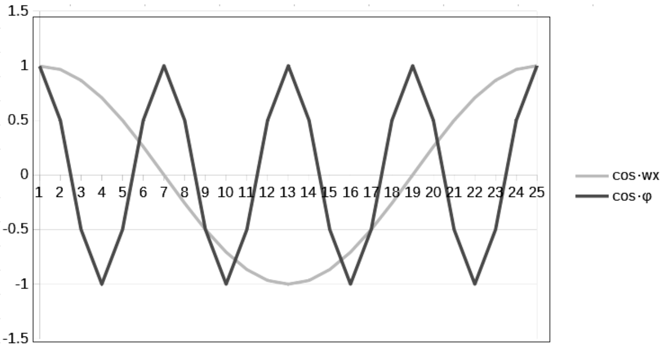
Then we set cosine curves as the wave functions $\cos wx$ for the Hamiltonian equation (4). Also, we set $\cos\varphi$ to model the photon's wave function, where frequency of $\cos\varphi$ is higher than of $\cos wx$ as shown in Fig. 3.



(1) r: distance of an electron from the origin



(2) R: distance between two protons



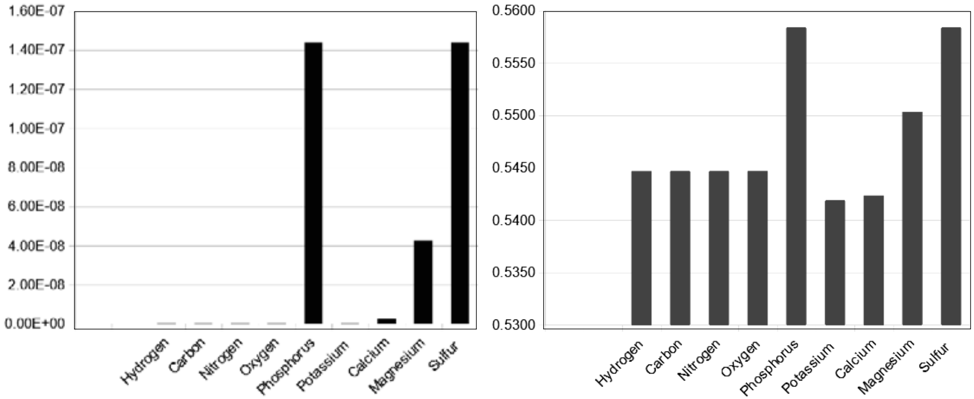
(3) cos·wx and cos·φ

Fig. 3 Input data for the simulation: R, r, cos·wx and cos·φ

Input data for the numeric simulation. Then the input data were made on R, r, $\cos wx$ and $\sin wx$ as shown in Fig. 3. The case of $\sin wx$ was also calculated during this research, but it was eliminated from this report due to the less significance of the calculated standard error of the coefficient.

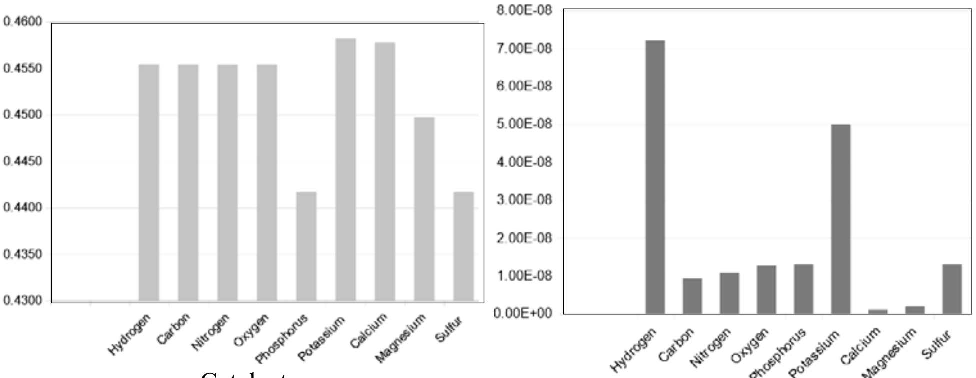
RESULTS AND DISCUSSION

Fig. 4 and Fig. 5 illustrate the outcomes of the calculations that uncover the probabilities of energy transitions between atoms through distinct mechanisms: elastic scattering, charge exchange, catalysts, and photosynthesis. We will focus on the latter three mechanisms, as elastic scattering involving protons is found to be negligible.



Elastic

Charge exchange



Catalyst

Photosynthesis

Fig. 4. Probabilities of Elastic Scattering, Charge Exchange, Catalyst Perturbation, and Photosynthesis

Early Stage of Wheat/Maize Growth. The insights from Fig. 4 are interesting. They suggest that Nitrogen (N), Hydrogen (H), and Oxygen (O) atoms have a unique connection with enzymes, driven by electrostatic energy. This observation holds significance during the initial stage of wheat and maize growth. At this juncture, enzymes like glutamate synthetase (GS), a pivotal role in converting inorganic compounds such as ammonium (NH_4^+) and nitrate (NO_3^-), into organic compounds like glutamate ($C_5H_9NO_4$). These compounds lay the foundation for the plant's structural development.

Latter Stage of Wheat/Maize Growth by Photosynthesis. Advancing with Fig. 4, we find Nitrogen (N) taking a central role in the adiabatic charge exchange process, shaping the plant's main body. Enzymes also contribute to this process, collaborating with Nitrogen (N). Photosynthesis, however, appears to have a gentler effect on Nitrogen (N), but exerts a more prominent influence on non-enzyme atoms like Potassium (K). This balance reflects the rhythms of nature: photosynthesis becomes significant after the plant has established its protein structure, while the enzyme-driven charge exchange process takes precedence in earlier stages.

Fermentation Process for Biogas Production. Moving beyond growth stages to the biogas production, Fig. 4 extends its narrative. It emphasizes the significant roles of adiabatic charge exchange and enzyme activity in transforming substances into methane (CH_4) and carbon dioxide (CO_2). Interestingly, photosynthesis, which often occupies a prominent position in energy discussions, appears to exert a subtler influence in the context of fermentation. These insights deepen our understanding of how plants harness and covert energy.

Common Patterns. Revealing broader patterns, this study consistently emphasizes enzyme atoms as key players in the adiabatic charge exchange process. This observation waves a coherent thread through the narrative: the orchestrated absorption of Nitrogen (N) from the soil, contributing to the formation of plant structures. Additionally, the impact extends beyond enzymes. Catalysts, which are enzymes, also affect non-enzyme atoms like Potassium (K), Calcium (Ca), and Magnesium (Mg), showing nature's synchronized efforts to assimilate Nitrogen (N) into plant bodies. For example, the calculated probabilities of the adiabatic perturbation and the electrostatic perturbation on the atoms of Nitrogen (N), Hydrogen (H), and Oxygen (O) inspire possibilities of applying this result for further making other enzymes that may enhance the nitrogen assimilation process.

Table 2. Calculated results and the facts (discussions)

Stage of growth	Calculated probabilities in Fig. 4	Facts
The early stage of wheat/ maize growth	Each of Nitrogen (N), Hydrogen (H), and Oxygen (O) have the high probability of catalyst perturbation. It means the enzyme works well with these atoms, of the electrostatic energy.	During the early stage of wheat/maize growth, one of the enzymes, glutamate synthetase (GS), helps convert inorganic compounds, such as ammonium (NH_4^+) and nitrate (NO_3^-), into organic nitrogen forms like glutamate ($C_5H_9NO_4$), which will be the main body of the plant.
Latter stage of wheat/ maize growth by photo synthesis	1. Nitrogen (N) has the high probabilities of the adiabatic charge exchange and the enzyme-catalyst reactions. 2. However, the probability of photosynthesis is negligible. 3. On the other hand, one of the non-enzyme atoms (in the plant body protein), Potassium (K), has the high probability of photosynthesis.	1. The main body of the plant is formed with the help of enzymes. 2. The photosynthesis should be effective only after the plant forms its protein structure. [Biol Res 43: 99-111, 2010 BR] 3. This result is also consistent with the fact that the photosynthesis should be effective in forming the plant's protein structure, while the enzyme is to enhance the photosynthesis of the plant proteins.
Fermentation	The probability of the catalyst perturbation is high on Carbon (C), Hydrogen (H), and Oxygen (O), which form methane (CH_3) and carbon dioxide (CO_2). The probability of adiabatic charge exchange is also large on these atoms	Fermentation process in biogas production from wheat and maize involves a series of physical reactions facilitated by various groups of microorganisms, leading to the generation of biogas, which is primarily composed of methane (CH_4) and carbon dioxide (CO_2).
Conclusion	The calculated results suggest that Nitrogen is notably influenced by adiabatic charge exchange and the enzyme-catalyzed reactions.	"Nitrogen fixation" is facilitated by enzymes and proteins through an adiabatic process without the need for heating, accompanied by photon absorption, which enhances the formation of robust protein structures.

CONCLUSION AND RECOMMENDATION

In light of the comprehensive investigation into the mechanisms governing the binding of Nitrogen (N) atoms to enzyme molecules and their implications for protein formation in food crops and biogas production, several key insights emerge.

Enhancing Protein Formation in Food Crops: The study's findings shed light on the intricate interactions occurring during the early and latter stages of wheat and maize growth. The high probabilities of catalyst perturbation, as indicated by the analysis, suggest that enzymes effectively collaborate with Nitrogen (N), Hydrogen (H), and Oxygen (O) atoms. Particularly during the initial growth stages, enzymes such as glutamate synthetase (GS) facilitate the conversion of inorganic compounds into organic nitrogen forms like glutamate, which contributes to the formation of the plant's structural components. These insights not only deepen our understanding of protein formation but also hold potential for optimizing crop growth strategies.

Biogas Production Optimization: For the fermentation process aimed at biogas production, the observation highlights the important role of enzyme atoms in both the adiabatic charge exchange process and the catalytic effects of enzymes in promoting methane (CH_4) and carbon dioxide (CO_2) production. These factors are crucial contributors to efficient biogas generation. Importantly, the limited influence of photosynthesis on the fermentation process suggests that the latter stages of plant growth are more relevant to biogas production. This understanding could aid in refining biogas production processes, potentially leading to increased energy yield from agricultural products.

Adiabatic Charge Exchange and Enzyme-Catalyst Dynamics: The research consistently highlights the role of the adiabatic charge exchange process, particularly concerning Nitrogen (N) assimilation into plant structures. This corresponds to the process of constructing the fundamental elements of plants by absorbing Nitrogen (N) from the soil. Additionally, the interplay between catalysts (enzymes) and non-enzyme elements such as Potassium (K), Calcium (Ca), and Magnesium (Mg) highlights how enzymes play a significant role in aiding the incorporation of Nitrogen (N) into plant structures, aligning with anticipated outcomes.

Ethical Consideration and Future Implications: Beyond the calculated results, these findings encourage us to ponder ethical dimensions. The concept of genetically enhancing enzymes for improved biogas production emerges as a guiding principle, as indicated by the Quantum Mechanics Approximation Approach. Unlike the heated debates surrounding genetic engineering in food crops this pathway appears to encounter fewer ethical challenges. The fusion of scientific understanding and ethical contemplation points to a fresh direction in optimizing biogas production.

Recommendation: As each calculated probability unveils the narrative of atomic interactions, the study's conclusions prompt us to take actionable steps. Guided by these insights, it is essential for the scientific community to initiate practical applications. Validating these findings through experiments in actual agricultural and biogas production settings could pave the way for transformative breakthroughs. Collaboration among mathematicians, molecular biologists, agricultural experts, and careful environmental management opens avenues to a future where mathematical analysis, innovation, and ethical considerations converge to address urgent needs in sustainable agriculture and renewable energy. In concluding this mathematical exploration, the symphony of intricate atomic interactions resonates. Beyond mathematical harmonic, we catch a glimpse of a world where ethical considerations intertwine harmoniously with exploration, guiding us toward a future enriched by mathematical inquiry, innovation and ethical guidance.

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Received 23.08.2023

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АПРОКСИМАЦІЙНИЙ ПІДХІД КВАНТОВОЇ МЕХАНІКИ ДЛЯ ДОСЛІДЖЕННЯ МОЛЕКУЛЯРНОЇ ПОВЕДІНКИ ЗВ'ЯЗУВАННЯ АЗОТУ З ФЕРМЕНТАМИ ТА БІЛКАМИ: ЗНАЧЕННЯ ДЛЯ ВИРОБНИЦТВА БІОПАЛИВА / Й. Мацукі, П.І. Бідюк

Анотація. Це дослідження заглиблюється у суттєві механізми зв'язування атомів азоту (N) з молекулами ферментів та їх наслідки для утворення білків у харчових культурах та виробництві біогазу. Азот, разом з фосфором (P) та калієм (K), відіграє важливу роль у родючості ґрунту та рості врожаю. Досліджено взаємодії між атомами за допомогою різних механізмів, таких як каталізатори, фотосинтез та адіабатичні реакції, для розуміння їх ролей у полегшенні утворення органічних молекул. Додатково досліджено вплив ферментів на амінокислоти та їх внесок у структуру білків. Процес симуляції використовує рівняння Гамільтона для кількісної оцінки інтенсивності енергії та дослідження ефективності адіабатичних реакцій у органічних перетвореннях. Через дослідження молекулярних взаємодій у фермент-каталізованих процесах це дослідження спрямоване на поліпшення утворення білків у врожаях та оптимізацію виробництва біогазу.

Ключові слова: зв'язування азоту, молекули ферментів, утворення білків, адіабатичні реакції, виробництво біогазу, утворення органічних молекул.