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Effect of Increased Molecular Force Attraction of NiO (Nickel Oxide) on the Kinetic and Potential Energy of H_2O Molecules for Efficient H_2O Splitting into H_2 Gas

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ABSTRACT

Nickel oxide (NiO) is a material used due to its remarkable chemical stability, magnetic properties, and electrical characteristics molecules. One notable feature of NiO is its unreactive surface with water (H2O), making it an ideal candidate for use as a cathode in the electrolysis process to produce hydrogen (H2) gas. During electrolyte process, H_2 is produced through the oxidation reaction at the anode and the reduction reaction at the cathode. Despite its potential, the detailed mechanism of H2O molecule decomposition using a NiO electrode remains inadequately explained. This research aims to elucidate the increased energy arising from the attractive forces between NiO and H2O molecules. To investigate these attractive forces, simulations were conducted to understand the chemical characteristics of the molecules, including bond lengths, bond angles, and their properties. The results indicated that the use of NiO electrode could increase the potential and kinetic energy of H_2O molecules. This energy increase is attributed to the formation of specific polar and non-polar bonds. Specifically, polar bonds were formed between (1) the nickel (Ni) atom in NiO molecules and the oxygen (O) atom in the H_2O molecules and (2) the O atom in NiO molecules and the H atom in the H_2O molecules. Non-polar bonds were formed between (1) the H atom in the H_2O molecules and the Ni atom in NiO molecules, and (2) the O atom in NiO molecules and the O atom in H_2O molecules. This study highlights how these interactions help in the electrolysis process by enabling the efficient breakdown of water molecules and the production of hydrogen gas.

Keywords: chemical characteristics, nickel oxide, non-polar, water splitting

1. INTRODUCTION

The electrolysis process involving the separation of water (H_2O) is a highly promising technique for converting renewable energy into hydrogen fuel (H_2) [1][2]. In this process, H_2 is produced through the oxidation reaction at the anode and the reduction reaction at the cathode [2][3][4]. Among the various cathode materials utilized, nickel oxide (NiO), a transition metal oxide, is one of the substances used due to its remarkable chemical stability, magnetic properties, and electrical characteristics [4][5]. Additionally, NiO is a cubic crystal that exhibits p-type semiconductor behavior with a bandgap energy of 3.6 to 4 eV at room temperature [6]. Previous research showed the significance of NiO, particularly as a thin film and as the cathode interface, in applications such as catalysis and energy production. Exploring the interaction of H_2O with metal substrates is an important topic in this context, and it can be investigated through quantum approaches, computer simulations, and experimental techniques. Molecular dynamics simulations are used to analyze the structure of H_2O at the metal oxide substrate interface [7]. Furthermore, there have been numerous analyses exploring the interaction of metal oxide-based semiconductors with H_2O, pioneered by the discovery of photoelectrochemical and catalytic phenomena exhibited by titanium dioxide (TiO_2) [8][9].

The presence of environmental humidity allows H_2O to form a coating on the metal oxide substrate, creating a substrate-like environment. Structural analysis of the H_2O molecules at the interface with the metal oxide substrate was carried out through a molecular H_2O modeling simulation approach [7]. Furthermore, the previous discovery of photoelectrochemical and catalytic phenomena in TiO_2 has prompted numerous investigations to analyze the interaction of metal oxide-based semiconductors with H_2O [8]. On metal surfaces, H_2O typically exhibits weak adsorption, similar to bulk ice, with binding energies being relatively low. However, this weak interaction becomes stabilized when directly bonded to the metal and H_2, enabling adjustments at the metal interface surface [10][11]. The interface between liquid and solid at the molecular level is a recent development in the field of surface science, occurring in various chemical, catalytic, electrochemical, materials science, and corrosion processes. These phenomena heavily rely on the behavior of particles, electrons, ions, and atoms [12].

The molecular modeling of H_2O is an important aspect of its molecular decomposition process [13]. For example, the molecular dynamics of H_2O can be observed when it comes into contact with an electrode surface [14][15]. The generation and evolution of gas resulting from this process are influenced by the surface hardness of both the electrode and porous solid surface [16]. In the case of NiO, it has been shown that the perfect surface does not react with H_2O unless there is oxygen (O) vacancy disassociation or when adsorbed O_2^- ions enhance reactivity at pre-oxidized surface defect sites [1][17]. However, there is no existing research discussing the increase in energy that occurs when NiO is used as an electrode catalyst for the decomposition of H_2O molecules. Therefore, this research aims to investigate the relationship between NiO and H_2O in terms of the energy increase resulting from the attractive forces between NiO and H_2O molecules.

In this research, the ChemDraw Ultra 12.0 software for molecular modeling to analyze the chemical characteristics of NiO and H_2O, including lengths, bond angles, and other relevant properties. Subsequently, the results of molecular dynamics, including essential parameters such as temperature, kinetic energy, potential energy, attractive forces, and their effect on the splitting of H_2O molecules into H_2 gas, were also analyzed using the HyperChem Professional software in a computational program.

2. RESEARCH SIGNIFICANCE

This research focuses on the intermolecular force attraction due to the influence of NiO molecules on H_2O molecules until H_2 atoms are detached from H_2O molecules. By understanding intermolecular attraction, we can identify atoms that are released from their bonds. The parameters affecting the release of hydrogen gas from H_2O due to NiO include force fields, dipole moments between atoms, kinetic energy, potential energy, temperature, and time. Specifically, in this research, the intermolecular force attraction between NiO and H_2O is directed to determine the concentration of hydrogen gas produced, which is utilized for environmentally friendly fuel applications.

3. RESEARCH METHODS

In this research, the materials analyzed are NiO and H_2O, with chemical structures NiO and H_2O. A molecular simulation method is employed using the computational device ASUS Notebook PC Processor Intel Core I5 5200 up to 2.7 GHz 4 GB. Several software are also used, including ChemDraw Ultra and HyperChem Professional Release for simulating the molecules, and Origin 8.5 software for visualizing graphical representations of the simulation results.

This research method is divided into two stages of simulation, namely:

A. Molecular characteristic data collection stage
B. The data collecting stage involve using molecular dynamics simulation and visualizing the data in a graphical form

3.1 Molecule Characterization Stage

The ChemDraw Ultra software is used to obtain the characteristics and properties of NiO and H_2O. The software structure menu is first opened, and the molecular structure name of NiO is entered. Furthermore, a 3-dimensional view is projected onto BioChem, which is integrated with ultra ChemDraw Ultra 12.0. The results obtained are data on the ratio of mass and total ionic charge, mass, and molecular weight, including the percentage content of nickel (Ni) and O components of NiO.

3.2 Simulation Stage of Molecule Dynamics

For drawing the structural forces of NiO and H_2O in a 3D view, Avogadro software is used. Hyperchem Professional 8.0 software is used to simulate energy enhancement in molecular dynamics simulations. In the computation menu, total molecular dynamics are selected to obtain the initial heating time and temperature of H_2O. Furthermore, molecular dynamics simulations are carried out to obtain data on kinetic energy, potential energy, and total energy, including temperature. The results of this energy data are then plotted in several graphs using Origin 8.5 64-bit software and analyzed.

4. RESULTS AND DISCUSSION

4.1 Molecular Characterization Stage of Nickel Oxide (NiO) and Water (H_2O)

The table below shows the molecular characteristics of NiO and H_2O obtained using the ChemDraw Ultra program.

Table 1. Characteristics of NiO molecules obtained from the ChemDraw Ultra program

Chemical formula	NiO
Molecular mass	73,93
Molecular weight	74,69
m/z	73,93 (100%)
Elemental Analysis	Ni; 78,58; O; 21,2
bond length	1.5394 A°

The data presented in the table shows that the molecular mass of NiO is higher than that of H_2O, affecting the bonding forces between the Ni atom in NiO and the H atom in H_2O. The H atom in H_2O detaches from its bond with the O atom due to the strong magnetic field interaction from NiO molecules [18]. This is caused by the strong atomic nucleus in the Ni atom, and the atomic nucleus is directly proportional to the molecular mass. The larger the molecular mass of a compound, the stronger its atomic nucleus [19].

Table 2. Characteristics of H_2O molecules obtained from the ChemDraw Ultra program

Chemical formula	H_2O
Molecular mass	18.01
Molecular weight	18.02
m/z	18.01 (100%)
Element analysis	H 11.9; O 88,81
Boiling point	291,08 K
Melting Point	166,45 K
Critical temperature	473,4 K
Critical pressure	80,58 Bar
Critical volume	45,5 cm^3/mol
Gibbs Energy	-135,32 kJ/mol
Henry's law	6,46

4.2 Molecular Dynamics Simulation Stage

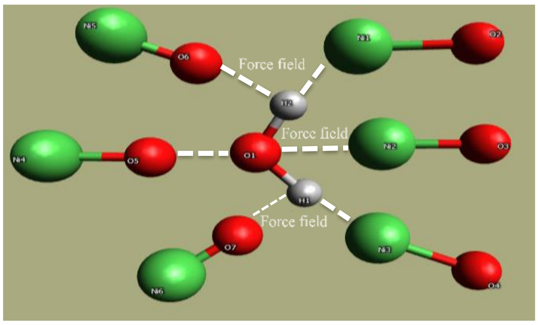

Fig 1. The atom configuration of the H_2O and NiO molecules as well as the force field between both compounds

Ni possesses a larger atomic nucleus and more protons than O, resulting in a gravitational attraction of O towards Ni nucleus. Therefore, Ni has a more negative charge compared to O. In other words, the O atom becomes more positively charged, leading to the formation of positive and negative poles, making the Ni atom in NiO molecules and the O atom in H_2O molecules polar or dipolar [20].The magnitude of the dipole compound is referred to as the dipole moment variable.

Fig. 1 shows that the Ni atom in NiO molecules forms an attractive polar force with the O atom in the H_2O molecules. Similarly, the O atom in NiO molecules forms an attractive polar force with the H atom in the H_2O molecules. The H atom in H_2O molecules forms a non-polar attractive force with the Ni atom in NiO molecules. The O atom in NiO molecules forms a non-polar attractive force with the O atom in the H_2O molecules.

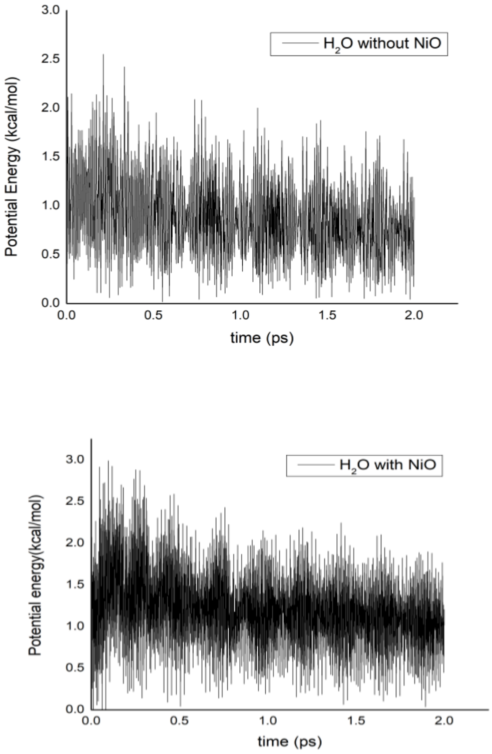

Fig 2. Graph of the potential energy of H_2O with and without the presence of NiO molecules

Fig. 2 shows the relationship between potential energy and time in H_2O molecules in the presence and absence of NiO. The graph shows that the potential energy of H_2O increases when NiO is present compared to when it is absent. The bond breaking of H_2O molecules exhibits a higher potential energy in the presence of NiO. Specifically, the potential energy values for H_2O with and without NiO are approximately 3.0 kcal/mol and 2.3 kcal/mol, respectively. The graph shows the up-and-down movement of the potential energy values, which is similar to the kinetic energy of the interaction between NiO and H_2O molecules. Furthermore, the pattern of motion between the two molecules affects the bond length and angle of the H_2O molecules.

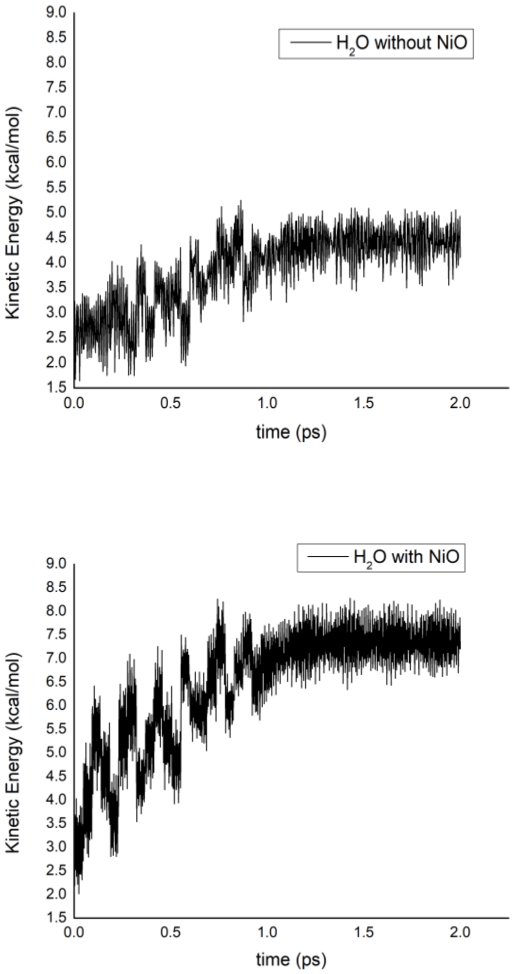

Fig 3. Graph of the kinetic energy of H_2O with and without the presence of NiO molecules

Fig. 3 shows the relationship between the kinetic energy of H_2O molecules over time, both with and without the presence of NiO. The graph indicates that there is a momentary change and a significant surge in kinetic energy. This phenomenon directly impacts the disruption of molecular bonds as molecules interact and exchange energy through collisions [21]. Therefore, the increase in molecular kinetic energy is accompanied by faster molecular motion. The graph also shows that the kinetic energy of H_2O molecules is higher in the presence of NiO compared to its absence due to the attractive forces between NiO and H_2O molecules [22]. From the H_2O with NiO graph, the maximum kinetic energy is about 6.5 kcal/mol after 0.1 ps. Meanwhile, the H_2O molecules without NiO reach a maximum kinetic energy of approximately 4.0 kcal/mol after 0.2 ps.

Figs. 2 and 3 shows the considerable threefold increase in the potential and kinetic energy of H_2O molecules when NiO is used as a cathode. This is a significant improvement, considering that the efficiency of H_2 gas evolution when NiO is applied as a photoelectrode currently reaches 28%. For H_2O molecules, when other molecules are present nearby, the dipole moment of H_2O molecules intensifies, although this approximation is not accurate enough for highly polar systems.

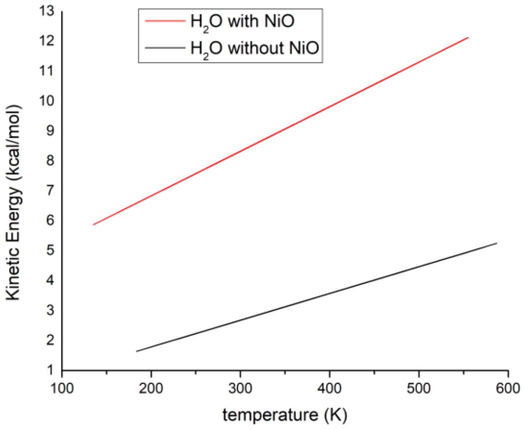

Fig 4. Kinetic energy of H_2O without and with the presence of NiO

Fig. 4 shows the relationship between the kinetic energy of H_2O with and without the presence of NiO molecules with respect to temperature. The graph shows that the kinetic energy of H_2O tends to increase as the temperature rises [23]. The kinetic energy for H_2O with and without the presence of NiO is approximately 7.5 kcal/mol and 4.7 kcal/mol, respectively, achieved at a temperature of about 500 K. This increase in kinetic energy is due to the forces between NiO and H_2O [24] [25], which influence the rate of H dissociation from H_2O [26]. This implies that when the kinetic energy value increases, the breaking of H_2O molecular bonds becomes more significant, leading to the splitting of H_2O molecules into H_2 gas [27]. The increase in kinetic energy is caused by the attractive forces between NiO and H_2O molecules, leading to improved conductivity and exhibiting NiO behavior as a semiconductor material.

Based on thermodynamic expectations, the behavior of H_2O in contact with NiO extends beyond the attractive forces between their molecules. To adequately understand this behavior, it is crucial to consider thermal fluctuations and various parameters such as temperature, volume, the number of particles, and the applied electric potential on NiO. Molecular dynamics simulations of H_2O with NiO surface can be conducted in two variations, either based on electronic structure theory or empirical force fields [10]. During this interaction, H_2O molecules undergo electron relocalization, resulting in atom density transfer that leads to an increase in potential energy but a decrease in kinetic energy. The increased density causes a decrease in potential and kinetic energy, stabilizing the molecules primarily due to changes in kinetic energy associated with the reduction in the density of nearby nuclei [28]. As a result, the changes in electron density, which are more concentrated in the core region, are relatively small. On the other hand, the changes in kinetic and potential energy are significant. This is because the increase in kinetic energy is dominated by the perpendicular bonding portions of the atoms [29]. As the percentage of NiO increases as an electrocatalyst, the potential variation indicating the change in cathode potential depends on the concentration of NiO [30].

5. CONCLUSIONS

In conclusion, as the molecular mass increases, the strength of atomic nuclei also increases, resulting in a stronger generated force field. In the configuration of interatomic force fields, NiO and H_2O tend to form polar compound units. This is reinforced by the presence of polar bonds between the Ni atom in NiO, the O atom in the H_2O, and the O atom in NiO with the H atom in H_2O. The formation of a polar compound leads to an increase in both kinetic and potential energy, enabling the atoms within the molecules to move rapidly and detach easily. High temperatures, which lead to increased kinetic energy, also play a role in breaking the bonds between the atoms. Therefore, the dissociation and combination of atoms of the same kind can result in the formation of H_2 and O_2 gases.

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7. AUTHOR CONTRIBUTIONS

Conception and design: Achmad Walid
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Resources, technical and material supports: Nurhadi
Supervision: Lisa Agustryana

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