Theoretical study of nickel-doped zinc oxide interaction with methylene blue and methyl orange using DFT methods

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Abstract

In this research, the adsorption of methylene blue (MB) and methyl orange (MO) on ZnO and nickel-doped ZnO (Ni-ZnO) clusters was investigated through the density functional theory (DFT). The study included the interaction with ionized MB, neutral MB, ionized MO and neutral MO. In the case of Ni-doped ZnO, the two probabilities of nickel multiplicities (1 and 3) have been included in the investigation. The interaction between water and ZnO cluster as well as water with Ni-ZnO multiplicity 1 and multiplicity 3 was also studied. The results showed that nickel doping can decrease the bandgap 25.38% which is promising to shift the UV source to the visible range in the photocatalytic process. For photocatalyst application it will bring the more benefit because it requires the lower energy. Moreover, the nickel doped induce the dye adsorp stronger when the dye attached to directly the zinc ion. This guide to design the N-doped ZnO photocatalyst with no nickel atoms on the surface of the photocatalyst.

1. Introduction

Solar energy is one of the most abundant sources of environmentally friendly energy, with a spectral component that consist of ~4% ultraviolet, ~46% visible, and ~50% near infrared light [1]. Solar energy can be used as a source to induce chemical reactions through photocatalytic processes. Many materials can be used as a photocatalyst, including TiO2 [2], CdS [3], ZnO [4], and Bi2WO6 [5]. Among the various materials, TiO2 and ZnO are the most widely used as photocatalysts. TiO2 has a bandgap similar to that of ZnO (3.20 eV), but the absorption efficiency of ZnO is larger than that of TiO2 in most solar spectra [6]. In addition, ZnO is considered to be a non-toxic metal oxide [7] and its production cost is relatively low [6]. However, ZnO’s photocorrosion issues and wide bandgap can limit its performance because it only absorbs light in the ultraviolet region and accelerates electron-hole pair recombination [8]. Metallic or non-metallic doping of ZnO can significantly overcome the disadvantages of ZnO by lowering the bandgap, thereby increasing the ZnO response to the visible light region. Several reports related to doping using alkali [9], transition [10], and nonmetal [11] can reduce the bandgap, but doping with alkaline metals [9] did not show a significant difference in the bandgap change.

Doping using transition metals, such as nickel metal, can improve the performance of ZnO. Nickel ions (0.69 Å) have an ionic radius close to zinc ions (0.74 Å), so nickel ion can easily replace zinc ion in the ZnO crystal lattice causing distortion of the ZnO crystal lattice and shifting to the visible region [12]. In addition, nickel has good corrosion resistance properties [13], which make it suitable for doping ZnO in photocatalyst applications. Nickel doping on ZnO which is used to remove dye pollutants experimentally has been reported by several researchers. Kaneva et al. reported that the photocatalytic activity of nickel doped on ZnO was better for the degradation of malachite green pollutants than without doping when irradiated using visible light, but
increasing the nickel concentration can reduce its performance in degrading malachite green \[14\]. These results contrast with those reported by Jayswal et al, in which a 10% nickel concentration produced the best photocatalytic activity for the degradation of methyl orange (MO), while at a 3% concentration the performance was worse than that without doping \[15\]. This finding shows that the presence of doping can change the surface properties of the material which affects the chemical properties of the material and its performance in degrading pollutants. However, the fundamental explanation at the molecular level for this phenomenon has not been experimentally explained regarding the interactions that cause electronic changes with the electron transfer that occurs on the ZnO surface. Computational chemistry is a series of techniques used to study chemical problems through computers \[16\] at the molecular level that cannot be explained experimentally (with only limited observation of physical phenomena). One of the computational methods to explain experimental observations at the molecular level is density functional theory (DFT) \[17\], and the accuracy of DFT calculations depend on the selection of the basis set and the density functional \[18\].

In order to find the optimum conditions for material composite preparation and for photocatalytic process, we investigate the influence of the nickel in the nickel-doped ZnO (Ni-ZnO) system on the interaction of ZnO and cationic or anionic dyes using a computational chemistry approach. The dye pollutant models used in this study were methylene blue (MB), which represents a cationic dye model, and MO, which represents an anionic dye; these have with molecular weights of 320 g mol\(^{-1}\) and 327.3 g mol\(^{-1}\), respectively. Dyes will have different forms in solution based on the acidity: neutral and ionized as shown in figure 1 \[19, 20\]. Thus, in this study, both forms have been included. This study can be used to optimize the solution acidity condition during the photocatalytic process of Ni-ZnO for methylene blue and methyl orange. The two multiplicities of nickel also have been considered in this study. In addition, the interaction between ZnO and Ni-ZnO with water is also studied, because water is used as a solvent for these dyes and is involved in the mechanism of the photocatalytic reaction. The interaction study of the both dyes on the Ni-doped ZnO has not been yet reported.

2. Computational methods

The adsorption interactions among MB and MO with ZnO and Ni- ZnO clusters were studied using a computational approach. This approach is separated into three steps that were used in previous research \[21, 22\]. First, make a model of the structure to be studied. Second, perform geometry optimization of all models. Third, adsorption simulation was performed by combining dyes or water with ZnO or Ni-ZnO clusters. The ZnO cluster was obtained from the file coordinates reported by Chen et al\[23\], while a Ni-ZnO cluster was
created by replacing one zinc atom with one nickel atom in the optimized ZnO cluster. The MB and MO structures were created using chemsketch software. The system nomenclature in this study is displayed in table 1.

The geometry optimization was conducted using the LANL2DZ \[24\] basis set with the exchange-correlation function B3LYP \[25, 26\] using the ORCA 4.2 version \[27\] programs. The calculation using this method has been performed by the other researchers and obtain the good agreement with previous studies or experiments \[28–30\]. Visualization of the calculation was performed using Chemcraft b610b software package (https://www.chemcraftprog.com). The interaction between dyes and water with ZnO or Ni-doped ZnO clusters was studied in various orientations, and the most negative adsorption energy was chosen as the model for the interaction investigation. Calculation of the adsorption energy from the interactions was calculated using equation (1).

$$\Delta E = E_{\text{opt-interaction}} - (E_{\text{opt-ZnO}} - \text{Ni-ZnO}) - E_{\text{optimized dyes/water}}$$

where $E_{\text{opt-interaction}}$ is the electronic optimized energy of the system dyes or water attached to ZnO and Ni-doped ZnO, $E_{\text{opt-ZnO}}$ is the electronic energy of optimized ZnO or Ni-doped ZnO clusters respectively, and $E_{\text{optimized dyes/water}}$ is the electronic energy of optimized methylene blue, methyl orange, and water. Charge transfer between dyes or water with ZnO or Ni-doped ZnO was determined by the Lowdin charge calculation \[30\].

### 3. Results and discussion

#### 3.1. The optimized geometry

In this study, a ZnO cluster with 12 oxygen or zinc atoms was used, as reported by other researchers \[31–33\]. The (ZnO)$_{12}$ cluster is used because it has a stable geometry with a cage-like structure, and as a results, the (ZnO)$_{12}$ cluster geometry is a good precursor for studying doped-ZnO \[29\]. From the calculation, it was found that the average Zn-O bond length was $\pm 1.985$ Å with a Zn-O-Zn bond angle in the hexagonal plane of $116.440^\circ$, while in the tetragonal plane, it was $\pm 90.837^\circ$. These results agree with the results reported by Afshari \textit{et al} using the same method \[10\]. For the experimental results reported by Djouadi \textit{et al}, the length of Zn-O was $1.962$ Å \[35\]. Therefore, the optimized (ZnO)$_{12}$ cluster can be used as an interaction model because the calculation geometry results are close to the geometry of the ZnO structure in nature. The optimized (ZnO)$_{12}$ cluster can be seen in figure 2. The incorporation of nickel ion into the ZnO cluster distort the structure. Xue \textit{et al} explained that replacing a zinc ion with a nickel ion does not form new compounds, but replacement of a nickel ion can cause distortion due to an increase in mutual repulsion between the Ni$^{2+}$ ion polarization charges \[36\]. NiI ZnO has more structural distortion than NiI ZnO. The bond distance between the atom in positions 1 and 4 has changed from 1.985 Å in ZnO to 1.865 Å in NiI ZnO and only to 1.950 Å in NiI3ZnO. The dihedral angle between atoms 2-1-3 changes from 123.75$^\circ$ in ZnO to 151.25$^\circ$ in NiI ZnO and 122.49$^\circ$ in NiI3ZnO. The details of the optimized structure are summarized in table 2.

The geometry optimization results of ionized MB and MO dyes do not show any significant difference from the experimental data \[37–39\], as shown in table 3. The calculated infrared spectrum of both molecules as displayed in figure 3 also in agreement with several literatures \[40–43\]. Based on this results, their optimized

| No | System name | Adsorbent | Adsorbate |
|----|-------------|-----------|-----------|
| 1  | ZnOMB0      | ZnO       | Neutral MB|
| 2  | ZnOMB1      | ZnO       | Ionized MB|
| 3  | ZnOMO0      | ZnO       | Neutral MO|
| 4  | ZnOMO1      | ZnO       | Ionized MO|
| 5  | ZnOW        | ZnO       | Water     |
| 6  | NiI ZnOMB0  | Ni-ZnO; Ni(II) multiplicity = 1 | Neutral MB|
| 7  | NiI ZnOMB1  | Ni-ZnO; Ni(II) multiplicity = 1 | Ionized MB|
| 8  | NiI ZnOMO0  | Ni-ZnO; Ni(II) multiplicity = 1 | Neutral MO|
| 9  | NiI ZnOMO1  | Ni-ZnO; Ni(II) multiplicity = 1 | Ionized MO|
| 10 | NiI ZnOW    | Ni-ZnO; Ni(II) multiplicity = 1 | Water      |
| 11 | NiI ZnOMO1  | Ni-ZnO; Ni(II) multiplicity = 3 | Neutral MB|
| 12 | NiI ZnOMO1  | Ni-ZnO; Ni(II) multiplicity = 3 | Ionized MB|
| 13 | NiI ZnOMO1  | Ni-ZnO; Ni(II) multiplicity = 3 | Neutral MO|
| 14 | NiI ZnOMO1  | Ni-ZnO; Ni(II) multiplicity = 3 | Ionized MO|
| 15 | NiI ZnOW    | Ni-ZnO; Ni(II) multiplicity = 3 | Water      |
structure of both dyes can also be used as an interaction model in this research. Meanwhile, the results of the optimized water molecule obtained a bond angle of 110° with an O-H bond length of 0.978 Å which is following that reported by Milovanovic et al [39].

3.2. Electronic properties of the ZnO and Ni-doped ZnO

The influence of nickel ion into the electronic properties of ZnO is in agreement with the previous report [44, 45]. The nickel ion cause the redshift to the ZnO band gap. The frontier molecular orbitals, HOMO and LUMO of ZnO, Ni1ZnO and Ni3ZnO are displayed in figure 4. Figure 4 shows that the HOMO is located in the oxygen position while the LUMO is located in the zinc position. This result is in agreement with a previous study [21]. HOMO describes an electron donor that shows the ability to donate electrons, while LUMO is an electron acceptor demonstrating the ability to acquire an electron. HOMO-LUMO represents the possibility of charge transfer in a molecule [46]. The nickel ion incorporation shifted the HOMO location to the nickel side. The shift

![Figure 2. The optimized structure of the (a) ZnO cluster, (b) Ni1ZnO cluster, (c) Ni3ZnO cluster. The grey balls represent zinc ions, the red balls represent oxygen ions and the green ball represents nickel ions.](image)

| System   | Distance* | Dihedral angle* |
|----------|-----------|-----------------|
|          | 1–2 (Å)   | 1–4 (Å)  | 1–3 (Å) | 2-1-4 (°) | 3-1-4 (°) | 2-1-3 (°) |
| ZnO      | 1,911     | 1,985    | 1,985   | 123,750  | 90,928   | 123,751   |
| Ni1ZnO   | 1,856     | 1,865    | 1,900   | 113,283  | 90,073   | 151,125   |
| Ni3ZnO   | 1,868     | 1,950    | 1,947   | 121,635  | 90,587   | 122,149   |

* Please see figure 2 for atomic number.

| Systems | Number of atom* | Calculation results (Å) | Experimental data (Å) | References |
|---------|-----------------|--------------------------|-----------------------|------------|
| MB1     | N7-C8           | 1.353                    | 1.340                 | [33]       |
|         | C8-C10          | 1.447                    | 1.440                 |            |
|         | S9-C10          | 1.814                    | 1.720                 |            |
|         | C10-C14         | 1.388                    | 1.350                 |            |
|         | C12-C14         | 1.435                    | 1.420                 |            |
|         | C12-N18         | 1.367                    | 1.330                 |            |
|         | N18-C20         | 1.479                    | 1.470                 |            |
| MO1     | N10-N11         | 1.295                    | 1.244                 | [34]       |
|         | C12-N11         | 1.426                    | 1.440                 |            |
|         | C6-N10          | 1.426                    | 1.407                 |            |
|         | C12-C16         | 1.415                    | 1.380                 |            |
|         | C15-C17         | 1.400                    | 1.390                 |            |
|         | S18-O20         | 1.649                    | 1.451                 |            |
|         | C13-S18         | 1.897                    | 1.780                 |            |
|         | C1-N7           | 1.399                    | 1.365                 |            |
|         | N7-C9           | 1.464                    | 1.446                 |            |

* Please see figure 2 for atomic number.
is more significant in the case of Ni1ZnO compared to Ni3ZnO. The difference in the values of HOMO and LUMO in Ni1ZnO is larger compared to the Ni3ZnO as shown in table 4. As a result, Ni1ZnO has the smallest bandgap among the three observed systems. The DOS of the three systems, as shown in figure 5, confirms that there are new states in Ni1ZnO that make the band gap narrower. These results are consistent with those reported by Pipornpong et al [11], where the HOMO position for ZnO is found throughout the atom, while during doped with nickel is around the nickel atom as well as for the LUMO position around the nickel atom. The bandgap results reported by Pipornpong et al are also similar to the calculation results as shown in table 4. The bandgap of low-spin nickel (multiplicity 1) is smaller than the high-spin (multiplicity 3), so this difference can make Ni-ZnO as a material used as a photocatalyst.

3.3. Investigation of the dyes or water interaction with ZnO or Ni-doped ZnO clusters
The placement of the dyes on ZnO or Ni-doped ZnO in the interaction study was done by considering the HOMO-LUMO profile of each molecule. The largest loop in the HOMO state will bind to the electrophile molecules. In the previous section it was reported that the ZnO cluster has a HOMO state around the oxygen ion so that the zinc ion was used to bind with the nucleophilic side of the dyes or water. Table S1 and S2 summaries the three possible positions of MB and ionized MB gathered with their adsorption energy calculation. There are three possible positions, first zinc ion of the ZnO binds to the sulfur of MB or ionized MB and the others are bind
to the nitrogen of MB. The adsorption energy calculation shows that the position 2 is the most preferable position for MB or ionized MB because they have the most negative value. Based on this result, we continued to use this position for the Ni-ZnO investigation system.

The investigation of the Ni-ZnO interaction with the dyes was conducted by varying the possible surface side starting from the interaction with nickel ion and moving far away from it, as displayed in figure S1. The energy adsorption calculation shows that the system in which dye binds to zinc ion is more preferable than the system that binds to the nickel ion (table S3-S7). This trend is observed for all adsorbates: MB, MB1, MO and MO1. This result gives a recommendation to design a composite material such that the dyes cannot directly interact with the adsorbate, for example, cover the surface with the ZnO layer to the Ni-ZnO.

The adsorption energy of the all-model system was calculated and the system which has a most negative energy adsorption is presented in table 5. A value that has a more negative value indicates a preferable system. Table 5 shows that the nickel ion in the Ni-ZnO induced the more negative adsorption energy, which also indicates the stronger adsorption. The presence of nickel ion in the ZnO system makes the zinc ions have the more positive the Lowdin charge. The more positive the Lowdin charge of zinc ion, the higher the charge difference between zinc ion and oxygen atom. The ionized dyes show a more negative adsorption energy.

Figure 4. The HOMO and LUMO of ZnO (a,b) Ni1ZnO (c,d) and Ni3ZnO (e,f) with an iso-value of 0.025.

Table 4. The HOMO and LUMO energy level of ZnO, Ni1ZnO, Ni3ZnO.

| System                        | HOMO (eV) | LUMO (eV) | Band gap (eV) |
|-------------------------------|-----------|-----------|---------------|
| ZnO                           | −6.738    | −2.711    | 4.027         |
| Ni-ZnO multiplicity 1         | −5.934    | −2.929    | 3.005         |
| Ni-ZnO multiplicity 3         | −6.665    | −2.708    | 3.957         |

The HOMO and LUMO of ZnO (a,b) Ni1ZnO (c,d) and Ni3ZnO (e,f) with an iso-value of 0.025.
compared than the neutral dye due to the more negative the Lowdin charge of oxygen in the MO. For the MB, different binding mode is observed for ZnOMB0. This difference explains why the ZnOMB0 has less adsorption energy than the others. In ZnOMB0, the dye interacts with ZnO through binding between hydrogen atom and zinc ion. In the others system, the dye interacts with ZnO through the binding between oxygen atom and zinc ion.

Figure 5. The DOS (density of states) of (a) ZnO, (b) Ni1ZnO and (c) Ni3ZnO.
When the MB was ionized, additional binding between hydrogen atom from dye and oxygen ion from ZnO was observed, even though this binding was weaker due to the longer distance. The effect of nickel ion multiplicity shows that nickel ion with multiplicity 1 (Ni1) has a more significant effect than nickel ion with multiplicity 3 (Ni3). The adsorption energy of the Ni1 systems show the more negative compared to the Ni3 systems. This result was also supported by the higher charge transfer that occurred in the Ni1 systems compared than in the Ni3 systems. Overall, Ni1MO1 is the most preferable system for the adsorption process. Experimentally, the result will show the different result due to the difference properties of the adsorbate.

4. Conclusion

In summary, the effect of nickel doped into ZnO to the MB and MO adsorption was investigated. The attachment of the dye with the nickel ion is less preferable than that with the zinc ion. This result guides the coating of the surface with a thin layer of ZnO after doping with the nickel ion. Incorporation of nickel ion into the ZnO also strengthens the adsorption. Overall, ionized MO shows the strongest adsorption on the Ni1ZnO surface. This research can be used to optimize the condition during the photocatalytic process Ni-ZnO for methylene blue and methyl orange with pH. Adsorption can become optimum for methyl orange when the pH of the solution > 3.8, while methylene blue can be optimum at pH > 6.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

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