UNDERSTANDING INSIGHT OF METHANOL ADSORPTION ON 2 ATOMIC COPPER DEPOSITED OVER ZNO($10\bar{1}0$) SURFACE: A DFT STUDY

VO THANH CONG, NGUYEN VAN SON, PHAM THANH TAM
Faculty of Chemical Engineering, Industry University of Hochiminh City, Ho Chi Minh City, Viet Nam
nguyenvanson@iuh.edu.vn

Abstract. In this study, depositing with two copper atoms (2Cu) on ZnO($10\bar{1}0$) surface, obtaining 2Cu/ZnO($10\bar{1}0$) surface model, and its applications then for adsorbed CH_3OH were investigated using the density functional theory (DFT). In performances, 2Cu was adsorbed on ZnO($10\bar{1}0$)surface to form the model of 2Cu deposited over ZnO (2Cu/ZnO). Further, on 2Cu/ZnO surface model, the resulted analysis as density of state (DOS) and electron density difference (EDD) contour plot pointed out that two atomic Cu were formed by the transferred electrons from Cu to ZnO, leading Cu oxidation to become Cu^+ ion, while was modeled 2Cu/ZnO($10\bar{1}0$)surface. To investigate CH_3OH adsorption, many configurations of adsorbed CH_3OH on the surface found, in which the most stable configurations were also identified. This result presented that methanol adsorption on 2Cu/ZnO is more favorable than that on ZnO in our previous works.

Keywords. DFT, DOS, EDD, 2Cu/ZnO, CH_3OH adsorption

1. INTRODUCTION

In recent year, alternative energy resource has become a hot issue because of energy crisis. If we can't develop new energy supply, the conventional fossil fuel source will be completely exhausted in fifty years. Hydrogen energy, considered as one of the relative energies, receiving highly attention since it is environmental-friendly, widely-available and it has high conversion efficiency[1, 2]. Hydrogen is never found alone on earth, it is always combined with other elements such as oxygen and carbon. Hydrogen can be extracted from virtually any hydrogen compound and is the clean energy carrier. In industry, hydrogen source can be produced from any compounds such water and organic hydrocarbon compounds and used as renewable energy resources in which it has fact that received increasing attention recently is undeniable [3, 4]. Today, hydrogen is primarily used as a feedstock in the chemical industry, for instance, ammonia manufacture, petroleum refinement and methanol synthesis[1, 5]. Therefore, considering hydrogen's potential contribution to the development of an alternative fuel, it has been known as a key energy solution for the 21st century [1, 6, 7].

Methanol (CH_3OH) product is mainly prepared by synthesis-gas conversion which it has an available in abundant feedstock and already largely distributed. Methanol has been known also such as renewable energy and to be a famous fuel for conversion to hydrogen [6, 8], because, it has an the advantages of being high H/C ratio, low sulfur content, and storage/dispense requirements[9, 10]. Therefore, the adsorption and dissociation to convert CH_3OH has mentioned great interests of researchers to what we performed in this works.

It has been reported in previous investigations [11-14] that Cu-based catalysts have often used for many chemical process such as water gas shift reaction, dehydration, methanol steam reforming, etc. In further, it has proven that the metal oxide of ZnO is with high Cu atom dispersed to form Cu-ZnO catalyst surface which given a higher conversion and selectivity [12, 15, 16]. As a result, the target study of two atomic Cu deposited over ZnO($10\bar{1}0$) (called as 2Cu/ZnO) are performed in this works. By doing this, it is confident that 2Cu/ZnO adsorbent can be used well for CH_3OH adsorption process. In addition, to understand the possible diffusion of two atomic Cu on the surface ZnO is stable or not, with the aim of improving adsorption properties for chemical reaction in next research. Simultaneously, a comparison of CH_3OH adsorption between Cu/ZnO and ZnO surfaces are performed also in this study.

It has been proved that DFT was theoretical techniques able to calculate the elementary reactions [15, 17, 18]. Consequently, we used here the DFT calculations to investigate CH_3OH adsorption on the

2Cu/ZnO($10\bar{1}0$) surface. In particular this investigation, many configurations of 2Cu adsorbed on ZnO surface, forming 2Cu/ZnO($10\bar{1}0$) surface model are considered to find the result of the most stable one. Hereafter, CH_3OH adsorption on this surface are examined then. Many adsorption configurations among the most stable one of CH_3OH adsorbed on 2Cu/ZnO($10\bar{1}0$) surface based on adsorption energies are determined and found. In addition, natural and characteristic bonds in interaction between 2Cu and ZnO surface are explained by the calculations of DOS and EDD contour plots, respectively.

2. COMPUTATIONAL DETAILS

All calculations on the basic of plan-wave periodic density functional theory using Vienna ab initio Simulation Package (VASP) code were performed. [19-21] The exchange correlation energy was treated within the generalized gradient approximation (GGA) using the shape of functional described by Perdew-Wang 1991(PW91) [22, 23]. The description of electron-ion interactions were used for the projector augmented wave (PAW) method [24], and we performed spin-polarized calculations for all of the structural optimizations. The calculations were carried out using the Brillouim zone sampled with (4×4×4) and (4×4×1) Monkhorst-Pack [25] mesh k-points grid for ZnO bulk and all of ZnO($10\bar{1}0$) surface calculations, respectively.

The optimized (2 x 2) unit cells of the most stable ZnO($10\bar{1}0$)surface with six layers were modeled as periodically repeating slabs, which similar to our previous work [10]. The top three layers were free to relax in the calculations of surface adsorption and interfacial reaction, and the bottom three layers were fixed at the computed lattice constants to represent the semi-infinite bulk crystal. In order to minimize the interaction between slabs in this infinitely periodic model system, a vacuum region of 15Å was introduced to prevent the interaction of slabs. The Kohn–Sham one-electron wave functions were expanded in a plane wave basis with a cutoff energy of 380 eV. Ionic relaxations were performed using the conjugate gradient method until the forces on all unconstrained atom were less than 2×10^{-3} eV/Å [4, 10, 16, 26].

All of energy equations are resulted in various cases of 2Cu deposited on ZnO($10\bar{1}0$)surface. The difference of initial structures is optimized and obtained. Considering possible adsorption sites of 2Cu adsorbed on ZnO surface, two kinds of adsorption energies are studied; the dispersion energy(E_{dispCu}) and surface energy(E_{Cu-ZnO}) equations were determined respectively, as follows,

$$E_{dispCu} = \frac{E_{nCu/slab} - (E_{slab} - nCu)}{n} \quad (1)$$

$$E_{Cu-ZnO} = \frac{E_{nCu/slab} - (E_{slab} - E_{nCu})}{n} \quad (2)$$

Where, $E_{nCu/slab}$, E_{slab} and E_{nCu} represent the dispersion energies of Cu on ZnO($10\bar{1}0$) surface, one cleaned ZnO surface, and one Cu in gas phase are adsorbed, respectively; n is number of the adsorbed Cu. A negative E_{dispCu}value referred a gain of energy concludes the thermodynamically favorable adsorption.

To calculate the adsorption energies of methanol on 2Cu/ZnO surface, the adsorption energy (E_{ads}) of adsorbate (methanol) and surface (2Cu/ZnO) system is defined generally equation as following.

$$E_{ads} = E_{adsorbate-surface} - E_{surface} - E_{adsorbate} \quad (3)$$

In which, $E_{adsorbate-surface}$, $E_{surface}$, and $E_{adsorbate}$ shown as interface energy calculation between the adsorbate and surface, one clean surface, and one molecule in gas phase are adsorbed, respectively. In addition, it is noted that all of adsorption energy values as minus sign to point out the energies are favorable in thermal systems.

3. RESULTS AND DISCUSSION

3.1. Surface model of 2Cu/ZnO

Depositing of 2 atomic Cu on ZnO surface is systemically calculated. Five adsorption configurations showing at figure 1, corresponding to the calculated adsorption energy of adsorbed 2Cu on the ZnO surface, namely from site I to site V are found and listed in Table 1 as follows.

Table 1: The dispersion adsorption energy per adsorbate ($\boldsymbol{E_{dispCu}}$), and surface energy ($\boldsymbol{E_{Cu-ZnO}}$) of 2Cu atoms adsorbed on ZnO($\mathbf{10\bar{1}0}$)surface.

Sites	E_{dispCu}, (eV)	$E_{Cu\text{-}ZnO}$ (eV)
I	-2.21	-0.96
II	-2.63	-1.10
III	-2.47	-1.15
IV	-2.48	-1.36
V	-2.59	-1.57

It is observed in Table 1 that the adsorption energy of site V is calculated with dispersion energy of -2.59 eV, and surface energy of -1.67 eV which it is larger than that from site I to site IV. This indicated that site V is the most stable one. Further, the adsorption configurations of all site from I to V are presented in Figure 1.

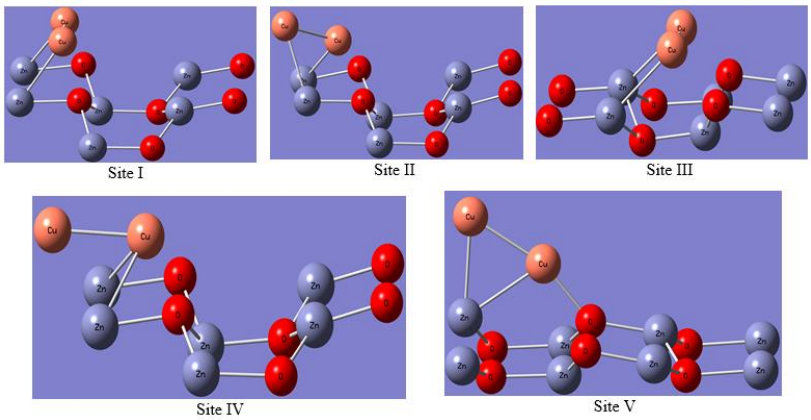


Figure 1. The side view of 2Cu adsorbed on ZnO $(10\bar{1}0)$ surface.

It is known to base on adsorption energy that the configuration of side view of site V is calculated as most stable site. Thus, the study of methanol adsorption will be focused on examination in this works. It is an observation at Figure 1 for site V, we find that one Cu atoms sits on top site of Zn toms with Cu-Zn distance of 2.15 Å. Whereas, another atomic Cu is bonded on both Zn and O atoms on the surface ZnO with Cu-O distance of 1.62 Å and Zn with Cu-Zn distance of 2.37 Å. In addition, finding at configuration in Figure 1 are showing that between 2Cu atoms and ZnO surface, formed a chain of Zn-O-Cu-Cu-Zn-O 'zigzag connection' which is Zn-O bond length of 1.85 Å shortened, and Cu-Cu bond length of 2.17 Å elongated. By this formation, 2Cu deposited on ZnO$(10\bar{1}0)$ surface has many active sites to methanol adsorption is more favorable to compare with ZnO only surface.

To understand the bond interaction between methanol molecule and 2Cu/ZnO$(10\bar{1}0)$ surface, a density of states (DOS) for site V are plotted in Figure 2.

It is an observation of DOS in Figure 2(a) that the states 2Cu atoms before (solid line) and after (short-dash line) adsorption decreased the electrons density at interval energy from -5 eV to 0 eV (Fermi level) after 2Cu adsorption, this indicated that electron in orbital of 2Cu donated to surface ZnO after adsorption. The electron donation formed a chemical bonding of methanol on the surface. Further, the observation of DOS in Figure 2(b), the states of ZnO surface before (solid line) and after (short dash line) adsorption is clearly that ZnO surface after adsorption decreased electron and shifted right at the Femi level, this shown electronic 2Cu donation to surface after adsorption. Herein, our calculations of DOS analysis is in line with previous investigation [27, 28], this follow us to make a confident data that 2Cu/ZnO surface model is obtained to be suitable. In further, through explaining DOS, it can conclude that Cu is oxidized to form Cu+ ion on the 2Cu/ZnO surface. This makes Cu to become thus more active after deposition on the surface ZnO.

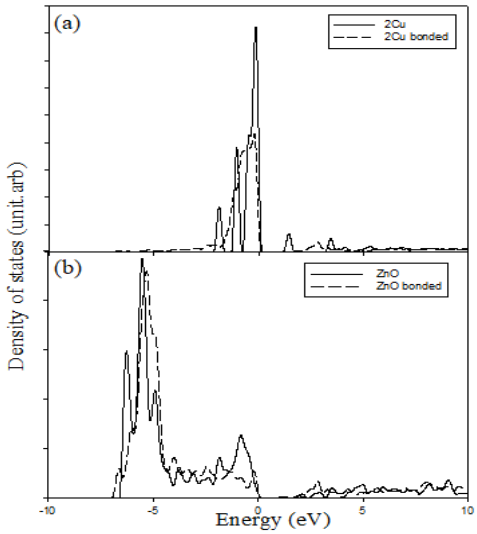
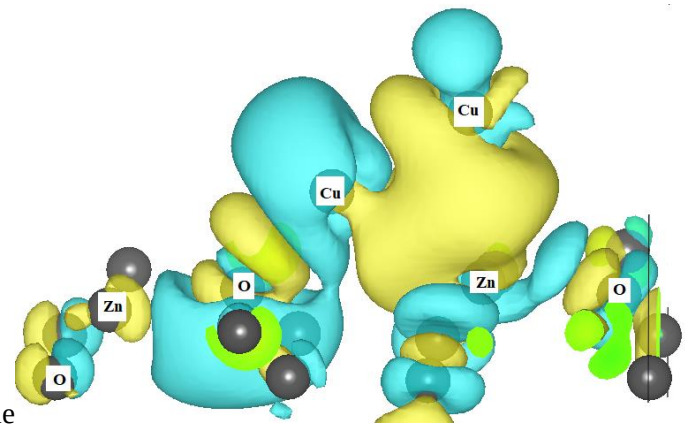


Figure. 2. DOS of 2Cu adsorbed on ZnO$(10\bar{1}0)$ surface. In which, Figure 2(a) is denoted as DOS analysis of 2Cu adsorption on the surface. Whereas, Figure 2(b) shown as DOS of ZnO after adsorption.

To understand more insight in adsorbed 2Cu on the surface, an electron density difference (EDD) was also plotted also in Figure 3.



able

Figure 3. EDD contour plot of 2Cu adsorption on 2Cu/ZnO surface. In which, the yellow-line is noted as electrons loss, and green-line as electrons accumulation

Continuously, it is observed the EDD states in Figure 3 that increase and decrease of electron density area (yellow-line) between Cu and Zn with Cu and O are appeared in each contour plot, which it given a consistent with trend of the binding energy to form chemical bonds. In particularly, the electron loss of 2Cu atoms (yellow line) to O and Zn on surface ZnO, are indicated that Cu donated electron to surface, these causes have done a shorten of Zn-O bond length. The electron loss is in line with Cu oxidation to form Cu^+ ion on the surface ZnO. Resulted analysis is of DOS and EDD given an agreement with previous work [29]. This help us one again to have a confident database in calculation of 2Cu deposited over ZnO surface model.

3.2. Methanol adsorption on 2Cu/ZnO

The performance of CH_3OH adsorption, many positions of methanol adsorption on 2Cu/ZnO $(10\bar{1}0)$ surface, in which there is 4 the positions of adsorption site are found and considered in this works. The parameters and energy of CH_3OH adsorption in Table 2, the configurations in Figure 4 are obtained and calculated, respectively, as follows,

Table 2. The bond length (R, in Å), bond distance (d, in Å), bond angle (∠, in degree), and adsorption energies (Eads, in eV) for CH3OH adsorption on 2Cu/ZnO $(10\bar{1}0)$ surface with different adsorption sites

Sites	R (C-H)	R (C-O)	R (O-H)	∠COH	d(Zn… O_{ad})	d(Cu...O_{ad})	E_{ads}
1	1.10	1.43	1.37	132.1	1.98	-	- 1.26 (-1.14)[a]
2	1.10	1.46	0.98	109.9	-	2.02	- 0.64
3	1.10	1.45	1.00	107.7	2.15	-	- 0.55
4	1.11	1.41	0.99	106.9	2.56 (Cu…H)		-0.11
				CH_3OH gas phase			
Ref.[30-32]	1.09	1.43	0.97	109.5	-	-	-

[a] The CH_3OH adsorption energy on ZnO $(10\bar{1}0)$ surface was calculated by Cong *et al* [10].

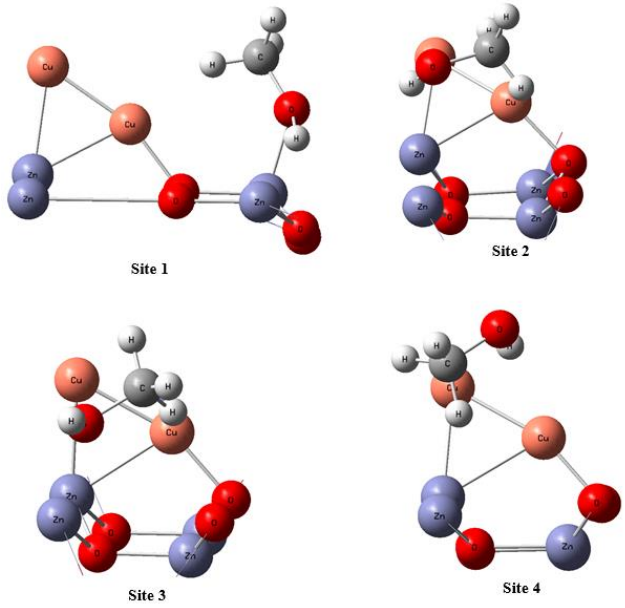


Figure 4. Configurations of CH3OH adsorbed on 2Cu/ZnO $(10\bar{1}0)$ surface at six different adsorption sites.

It is an observation in Table 1 that calculations of the general parameter and energy such as bond length, bond distance, and bond angle are changed after CH_3OH adsorption for comparison with CH_3OH in gas phase. This is to say that the interaction between CH_3OH molecule and the surface 2Cu/ZnO reacted together. We observe continuously the E_{ads} of site 1 (-1.26 eV) which this is the most stable one, whereas, site 4 to be the most unstable one (-0.11 eV). Herein, because the difference in interaction between methanol and the surface is that at site 1 (see in Figure 4) as O of methanol oriented to surface, whereas, site 4 to be oriented by H of methanol. As a result, the elongation of C-O and O-H bond length on site 1 become stronger interaction compare with that on site 4. Similar to that, site 1 is also more stable than from site 2 to site 4. Specially, we observed previous configuration of site 1 and site 2 in Figure 3 is that O of methanol bonding on site 2 oriented to interact with Cu on 2Cu/ZnO surface, whereas the O of methanol in site 1 is

to Zn. This is able to know that 2Cu/ZnO surface in which Zn active site adsorbed CH_3OH is better than Cu active site. Moreover, the E_{ads} value of site 1 on 2Cu/ZnO surface in this work is higher given than on ZnO only surface in our previous works [10], this indicated that the dispersion effects of 2Cu atoms to ZnO surface to which made atomic Zn of surface 2Cu/ZnO to be more active.

In addition, previous configuration of site 1 in Figure 3 is shown that CH_3OH adsorbed vertically on 2Cu/ZnO surface, where O bonded to Zn though the electrons transfer from lone pair of O in methanol. The bond distance of d ($Zn\ldots O_{ads}$) is found to be 1.98 Å (Table 2). The E_{ads} is calculated as -1.26 eV, C-O bond length of 1.43 Å and O-H bond length of 1.37 Å elongated, this value is much longer than from site 2 to site 5 to confirm that strong interactions between CH_3OH and 2Cu/ZnO surface on site 1 is found to be most stable adsorption configuration of methanol. Further, the geometrical parameters in this work are in good agreement with the experimental [30-32], which gives us more confident on method employed in this study.

4. CONCLUSIONS

The adsorption of CH_3OH on the 2Cu/ZnO($10\bar{1}0$) surface is investigated using the DFT method. The results of this works can be summarized as follows,

(1) Many sites of 2Cu deposited on ZnO($10\bar{1}0$) surface, formed 2Cu/ZnO($10\bar{1}0$) surface model. Based on dispersion and surface energies, site V is found to be the most stable one.

(2) DOS and EDD contour plot are analyzed on site V to provide the evidence of the high adsorption energies of 2Cu deposited on ZnO($10\bar{1}0$) surface, formed 2Cu/ZnO($10\bar{1}0$) surface model which 2Cu donated electrons to ZnO surface. This is to make 2Cu/ZnO surface to be more active than ZnO only surface.

(3) The calculated adsorption energies of CH_3OH adsorbed on 2Cu/ZnO, many site positions of adsorption configurations considered, in which the configuration of site 1 were found to be the most stable site.

This study explores the ability of Cu dispersion on ZnO($10\bar{1}0$) surface for the first time. Many calculations will be performed to go on the investigations such as Cu cluster improved on the surface or methanol decomposition reaction.

ACKNOWLEDGEMENT

We would like to thank to CPU time from Taiwan's National Center for High-performance Computing (NCHC) where supported this work is in the data calculations.

REFERENCES

[1] Y.-K. Lee, K.-S. Kim, J.-G. Ahn, I.-H. Son, W.C. Shin, Hydrogen production from ethanol over Co/ZnO catalyst in a multi-layered reformer, Int. J. of Hydrogen Energy, 35 (2010) 1147-1151.

[2] J. D. Holladay, Y. Wang, E. Jones, Review of Developments in Portable Hydrogen Production Using Microreactor Technology, Chem. Rev., 104 (2004) 4767-4790.

[3] A. Haryanto, S. Fernando, N. Murall, S. Adhikari, Current Status of Hydrogen Production Techniques by Steam Reforming of Ethanol: A Review, Energy & Fuels, 19 (2005) 2098-2106.

[4] K.-S.K. Yong-Kul Lee, Jin-Goo Ahn, In-Hyuk Son, Woo Cheol Shin, Hydrogen production from ethanol over Co/ZnO catalyst in a multi-layered reformer, International journal of hydrogen energy, 35 (2010) 1147-1151.

[5] A.C. A.J. Vizcaíno, J.A. Calles, Hydrogen production by ethanol steam reforming over Cu–Ni supported catalysts, International Journal of Hydrogen Energy, 32 (2007) 1450 – 1461.

[6] J.R. Wilson, G. Burgh, Energizing our Future: Rational Choices for the 21st Century, Wiley, Hoboken, NJ, 2008.

[7] Y.D. Kim, T. Wei, J. Stultz, a.D.W. Goodman, Dissociation of Water on a Flat, Ordered Silica Surface, Langmuir, 19 (2003) 1140-1142.

[8] J. Agrell, H. Birgersson, M. Boutonnet, I. Melian-Cabrera, R.M. Navarro, J.L.G. Fierro, J. Catal., 219 (2003) 389.

[9] M.D. Yan-Yan Chen, Zhangfeng Qin, Xiao-Dong Wen, Weibin Fan, Jianguo Wang, A DFT study on the adsorption and dissociation of methanol over MoS2 surface, Journal of Molecular Catalysis A: Chemical, 338 (2011) 44-50.

[10] C.T. Vo, L.K. Huynh, J.-Y. Hung, J.-C. Jiang., Methanol adsorption and decomposition on ZnO(1010) surface: A density functional theory study., Applied. Surface. Science., 280 (2013) 219-224.

[11] M.A.B. Orest Skoplyak, Jingguang G. Chen, Ethanol and ethylene glycol on Ni/Pt(111) bimetallic surfaces: A DFT and HREELS study, Surface Science 602 (2008) 3578–3587.

[12] J.H.L. Ann W. Grant, C. A. Perez,‡ S. Lehto, Martin Schmal, and Charles T. Campbell, Methanol Decomposition on Pt/ZnO(0001)-Zn Model Catalysts, J. Phys. Chem. B, 105 (2001) 9273-9279.

[13] S.B.H. S.A. Mirji, Nevin Mathew, V. Ravia, Nalini E. Jacob, K.R. Patil., Adsorption of methanol on Si(1 0 0)/SiO2 and mesoporous SBA-15, Colloids and Surfaces A: Physicochem. Eng. Aspects, 287 (2006) 51-58.

[14] Tetsuya Shishido, Manabu Yamamoto, Dalin Li, Yan Tian, Hiroyuki Morioka, Masahide Honda, Tsuneji Sano, K. Takehira., Water-gas shift reaction over Cu/ZnO and Cu/ZnO/Al2O3 catalysts prepared by homogeneous precipitation., Appl. Catal. A: General, 303 (2006) 62-71.

[15] F. Mehmood, J. Greeley, L.A. Curtiss, Density Functional Studies of Methanol Decomposition on Subnanometer Pd Clusters, J. Phys. Chem. C 113 (2009) 21789-21796.

[16] V.T. Cong, L.K. Huynh, J.-C. Jiang, N.T.A. Nhung, P.V. Tat, Density function theory study of water gas shift reaction on 2Cu/ZnO (10-10) surface, Computational and Theoretical Chemistry, 1081 (2016) 62-70.

[17] X. Wang, W.-K. Chen, C.-H. Lu, A periodic density functional theory study of the dehydrogenation of methanol over CuCl(111) surface, Appl. Surf. Sci., 254 (2008) 4421–4431.

[18] B. Meyer, D. Marx, Density-functional study of Cu atoms, monolayers, films, and coadsorbates on polar ZnO surfaces, Physical Review B, 69 (2004) 235420.

[19] G. Kresse, J. Furthmüller, Efficient iterative schemes for ab initio total-energy calculations using a plane-wave basis set, Phys. Rev. B, 54 (1996) 11169.

[20] G. Kresse, J. Furthmüller, Efficiency of ab-initio total energy calculations for metals and semiconductors using a plane-wave basis set., Comput. Mat. Sci, 6 (1996) 15.

[21] G. Kresse, J. Hafner, Ab initio molecular-dynamics simulation of the liquid-metal-amorphous-semiconductor transition in germanium, Phys. Rev. B, 49 (1994) 14251.

[22] J.P. Perdew, J.A. Chevary, S.H. Vosko, K.A. Jackson, M.R. Pederson, D.J. Singh, C. Fiolhais, Erratum: Atoms, molecules, solids, and surfaces: Applications of the generalized gradient approximation for exchange and correlation, Phys. Rev. B, 48 (1993) 4978.

[23] J.P. Perdew, J.A. Chevary, S.H. Vosko, K.A. Jackson, M.R. Pederson, D.J. Singh, C. Fiolhais, Atoms, molecules, solids, and surfaces:Applications of the generalized gradient approximation for exchange and correlation, Phys. Rev. B, 46 (1992) 6671.

[24] P.E. Blochl, Projector augmented-wave method, Phys. Rev. B, 50 (1994) 17953.

[25] H.J. Monkhorst, J.D. Pack, Phys. Rev. B, 13 (1976) 5188.

[26] V.T. Cong, D.Q. Diem, N.M. Quang, P.T. Tam, a.P.V. Tat, Co-adsorption of CO, H2O, and Mechanism of Water Gas Shift Reaction on ZnO Catalyst Surface: A Density Functional Theory Study, Vietnam Journal of Science and Technology 55 (2017) 95-104.

[27] B.T. Yun Zhao, Zongxian Yang, Yue Zhao, Leihong Zhao, and Mengfei Luo, Density Functional Theory Study of Sn Adsorption on the CeO2 Surface, J. Phys. Chem. C 115 (2011) 16461–16466.

[28] a.M.N. Ali Ahmadi Peyghan, Density Functional Study of the Adsorption of Methanol and Its Derivatives on Boron Nitride Nanotubes., Ali Ahmadi Peyghan and Maziar Noei/Adsorption Science & Technology., 31 (2013) 9.

[29] Y. Zhao, B. Teng, Z. Yang, Y. Zhao, L. Zhao, M. Luo, Density Functional Theory Study of Sn Adsorption on the CeO2 Surface, J. Phys. Chem. C, 115 (2011) 16461-16466.

[30] W.-K. Chen, S.-H. Liu, M.-J. Cao, Q.-G. Yan, C.-H. Lu, Adsorption and dissociation of methanol on Au(1 1 1) surface: A first-principles periodic density functional study, Journal of Molecular Structure: THEOCHEM, 770 (2006) 87-91.

[31] D.R. Lide, CRC Handbook of Chemistry and Physics, 81st., ed., CRC Press, Boca Raton, FL, 2000, pp. 9-36.

[32] Y.-Y. Chen, M. Dong, Z. Qin, X.-D. Wen, W. Fan, J. Wang, A DFT study on the adsorption and dissociation of methanol over MoS2 surface, Journal of Molecular Catalysis A: Chemical, 338 (2011) 44-50.

HIỂU SÂU SỰ HẤP PHỤ METHANOL TRÊN BỀ MẶT ZNO ($10\bar{1}0$) CÓ LẮNG ĐỌNG 2 NGUYÊN TỬ ĐỒNG: NGHIÊN CỨU MÔ PHỎNG DỰA TRÊN LÝ THUYẾT HÀM MẬT ĐỘ

Tóm tắt. Trong nghiên cứu này, hai nguyên tử đồng (2Cu) được lắng đọng trên bề mặt ZnO ($10\bar{1}0$), thu được kiểu bề mặt kiểu 2Cu/ZnO và được ứng dụng để hấp phụ methanol (CH_3OH) thực hiện dựa trên lý thuyết hàm mật độ (DFT). Chi tiết trong nghiên cứu, 2 nguyên tử đồng được lắng đọng trên bề mặt ZnO để hình thành kiểu bề mặt 2Cu/ZnO. Trong đó, bản chất liện kết trong sự lắng đọng của nguyên tử trên bề mặt ZnO được giải thích lần lượt thông qua tính toán của hàm mật độ trạng thái (DOS) và hàm mật độ sai biệt electron (EDD). Kết quả này chỉ ra rằng nguyên tử đồng nhường electron tới bề mặt ZnO, để nguyên tử Cu bị oxy hóa thành ion Cu^+. Trong nghiên cứu khả năng hấp phụ của CH_3OH trên bề mặt, nhiều cấu trúc của metanol hấp phụ trên bề mặt 2Cu/ZnO được thực hiện, trong đó cấu trúc bền nhất được tìm thấy. Các kết quả này thể hiện rằng, sự hấp phụ của CH_3OH trên bề mặt 2Cu/ZnO thì mạnh hơn trên chỉ bề mặt ZnO trong nghiên cứu của chúng tôi trước đó.

Từ khóa: DFT, DOS, EDD, 2 Cu/ZnO, CH_3OH adsorption

Ngày nhận bài: 02/12/2019

Ngày chấp nhận đăng: 25/03/2020