

# Theoretical Investigation of Fe and Al Surface Structure in the Case of H Adsorption using First Principles Calculation

N D Aisyah<sup>1,2,\*</sup>, D E Candrasari<sup>3</sup>, A Stefanus<sup>3</sup>, R Madinah<sup>3</sup>, R Nisa<sup>3</sup>, A H Zaidan<sup>3</sup>

<sup>1</sup> Research Center for Quantum Engineering Design, Universitas Airlangga, Surabaya 60115, Indonesia

<sup>2</sup> Department of Engineering Physics, Faculty of Industrial Technology, Institut Teknologi Bandung, Bandung 40132, Indonesia

<sup>3</sup> Department of Physics, Faculty of Science and Technology, Universitas Airlangga, Surabaya 60115, Indonesia

E-mail: nufidadwiaisayah@students.itb.ac.id

**Abstract.** This study reports the investigation of Fe and Al surface structure in the case of hydrogen adsorption. We vary the surface structure of both molecules based on the Miller index, cell area, and the number of layers. We use the Miller index of (100), (110), and (111). Then we vary the cell area of 2 x 2, 3 x 3, and 4 x 4, and the number of layers from one to four layers. We calculate the adsorption energy of hydrogen interacts to each different surface structure. The results show that four layers is enough to study hydrogen adsorption on Fe and Al surface. Meanwhile, the selection of the cell area is not necessarily considered.

## 1. Introduction

Most of the physical phenomena occurred involves the interaction with the surface. One of the phenomena is adsorption. [1] Adsorption occurs when an atom or molecule attached to the outer layer of the surface. [2]

The structure of the surface can be varied based on the Miller index, cell area, and the number of layers. The study of hydrogen adsorption on the Fe(100) and Fe(110) surface has been reported by Ferrin et al. [3] They calculated the adsorption energy using first principles calculation. Based on the study, they found that the adsorption energy obtained from the interaction of hydrogen and two different surface structure is different about 0.36 eV in the order of vibrational energy. This value is significant since the vibrational motion differs one system to another.

In this study, we attempt to investigate the effect of cell area and the number of layers on the adsorption energy of hydrogen on Fe and Al surface. We vary the Miller index of both surfaces. We use Fe(100), Fe(110), Fe(111), Al(100), Al(110), and Al (111). Each of the surfaces are varied by its cell area and the number of layers. All the variation of surface structure will be interacted to hydrogen atom using Density Functional Theory (DFT) scheme [4] to find the adsorption energy.

## 2. Computational detail

We model the adsorption using DFT. We perform all calculations using Quantum Espresso. We use the plane wave basis set and pseudopotential with PBE exchange-correlation. [5]

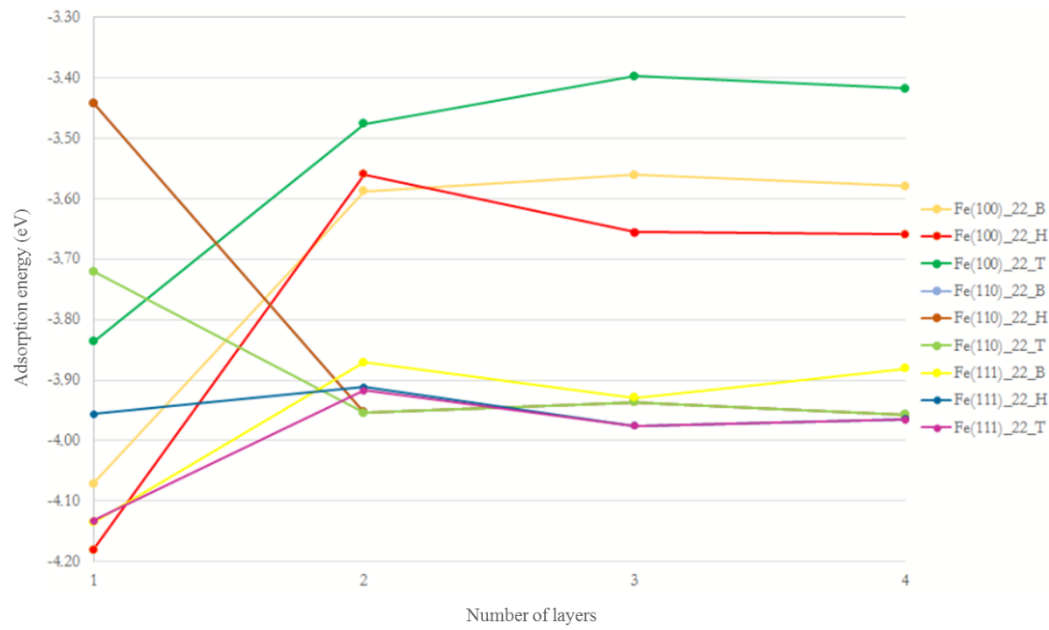
The adsorption energy can be obtained using the following formula. [6]



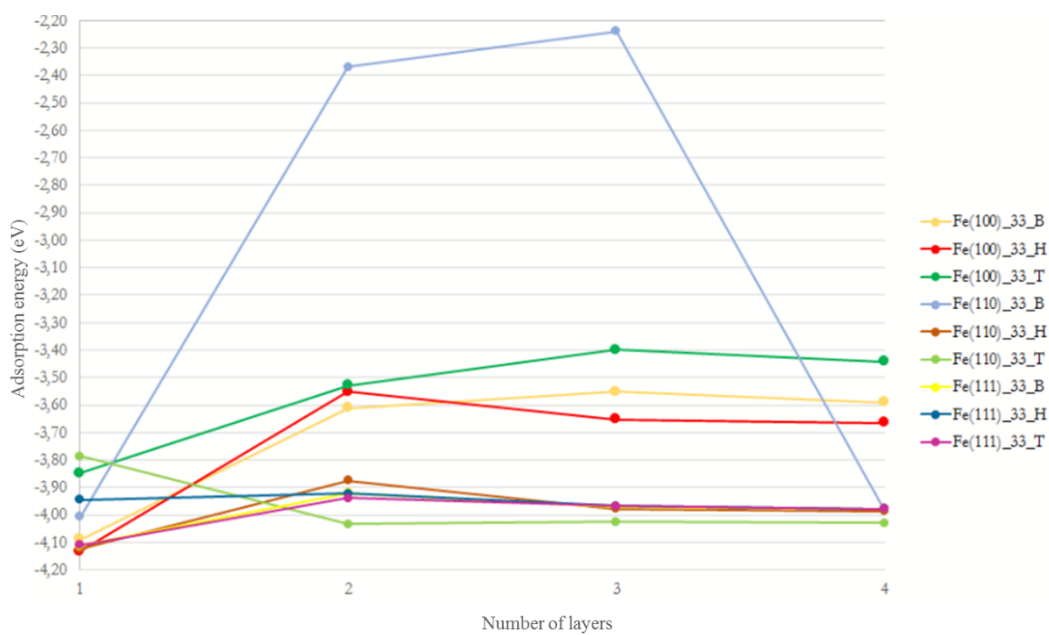
Content from this work may be used under the terms of the [Creative Commons Attribution 3.0 licence](https://creativecommons.org/licenses/by/3.0/). Any further distribution of this work must maintain attribution to the author(s) and the title of the work, journal citation and DOI.

$$E_{\text{adsorption}} = E_{\text{system}} - (E_{\text{surface}} + E_{\text{adsorbate}})$$

$E_{\text{system}}$  is the energy when the adsorbate, in this case is hydrogen, interact to the surface.  $E_{\text{surface}}$  and  $E_{\text{adsorbate}}$  are the ground state energy of surface and adsorbate respectively. The adsorption energy always results in negative values. It indicates the interaction occurs between hydrogen and surface.



(a)



(b)

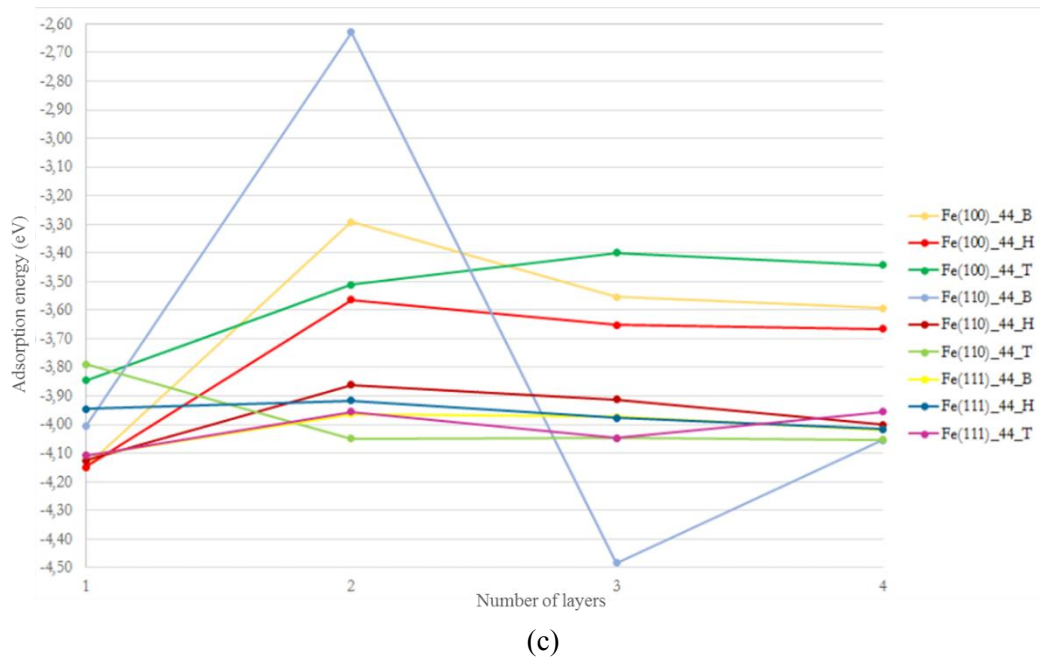


Figure 1. The adsorption energy against the number of layer of Fe with cell area (a) 2x2, (b) 3x3, and (c) 4x4.

We calculate the ground state energy of Fe and Al surface with three different miller index, (100), (110), and (111). The surface ( $n \times n \times l$ ) is varied by its cell area ( $n \times n$ ) and the number of layers ( $l$ ). We use  $2 \times 2$ ,  $3 \times 3$ , and  $4 \times 4$  cell area and one layers to four layers. The energy of the system is calculated by placing hydrogen atom on three different positions on the surface, bridge (B), hollow (H), and top (T). We plot the adsorption energy against the number of layers and the cell area to be analyzed.

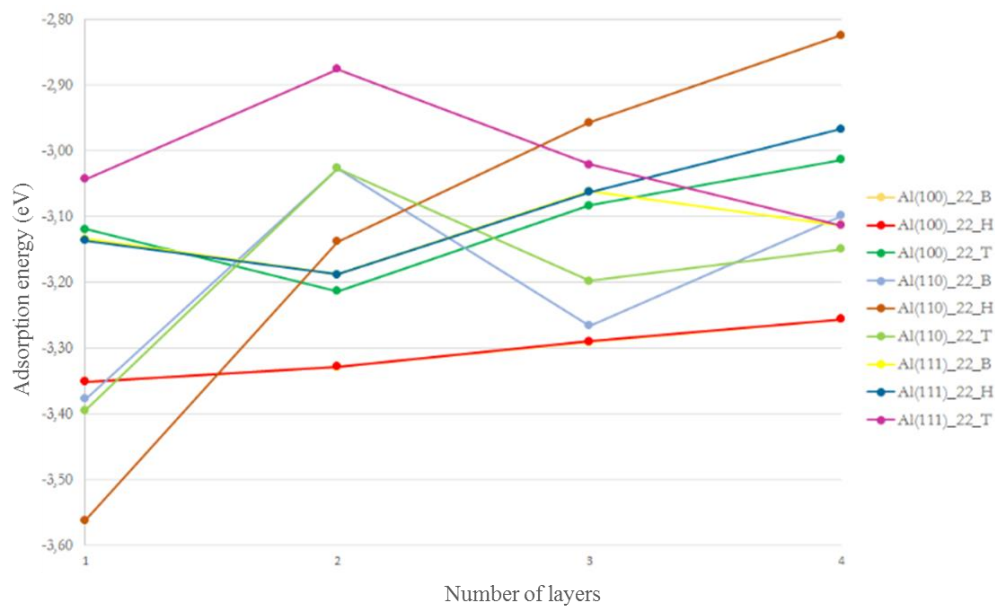
### 3. Results and discussion

#### 3.1. The effect of adding the number of layer

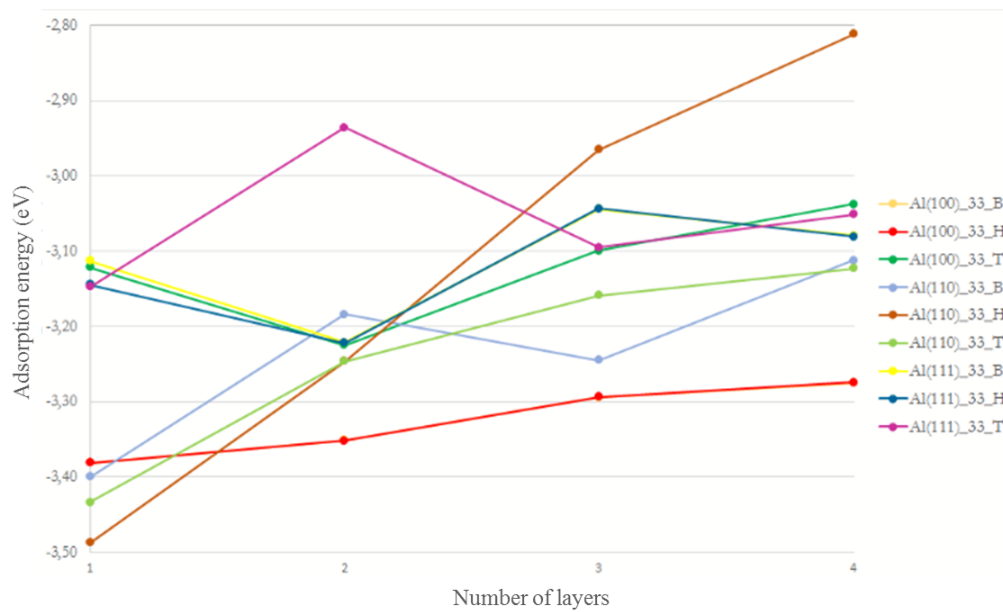
Figure 1 shows the effect of adding the number of the layer on Fe(100), Fe(110), and Fe(111) surface structure respectively on the adsorption energy in three different cell area,  $2 \times 2$ ,  $3 \times 3$ , and  $4 \times 4$ . For cell area  $2 \times 2$ , it shows that the significant changes of adsorption energy by adding one layer to two layers and it becomes insignificant from two layers to three layers and from three layers to four layers. The same trend occurs in another two cell area.

The significant changes in adsorption energy occur if the energy change is more than 0.1 eV. The reference of 0.1 eV comes from the minimum energy needed to change the vibrational state. The vibrational state influence the motion of atoms in the system. This motion differs one system to another. This motion differs one system to another. The significant changes when adding one layer to two layers occurs because of the more atoms contributes. Meanwhile, the insignificant changes occur because of the number of atoms contribute in the system is many, while the obtained adsorption energy is small. Thus the energy is not enough to influence the vibrational movement in the system. Thus Figure 1 indicates that four layers of Fe surface is enough to study the hydrogen adsorption.

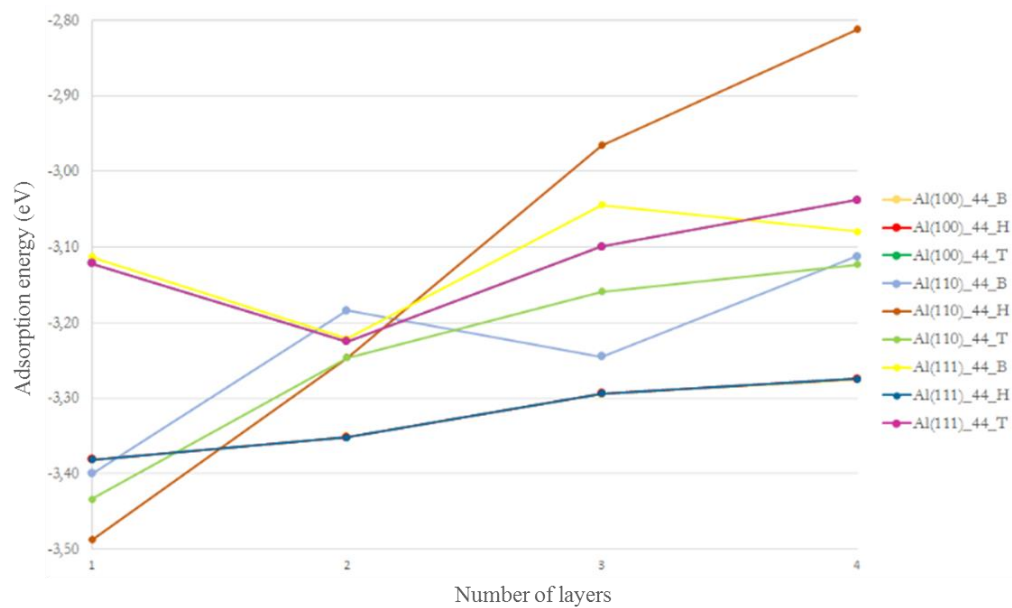
Figure 2 shows the same effect to Figure 1 but the effect occurs on Al surface. The same trend also occurs in all cell area. It indicates that four layers of Al surface is enough to study the hydrogen adsorption.



(a)

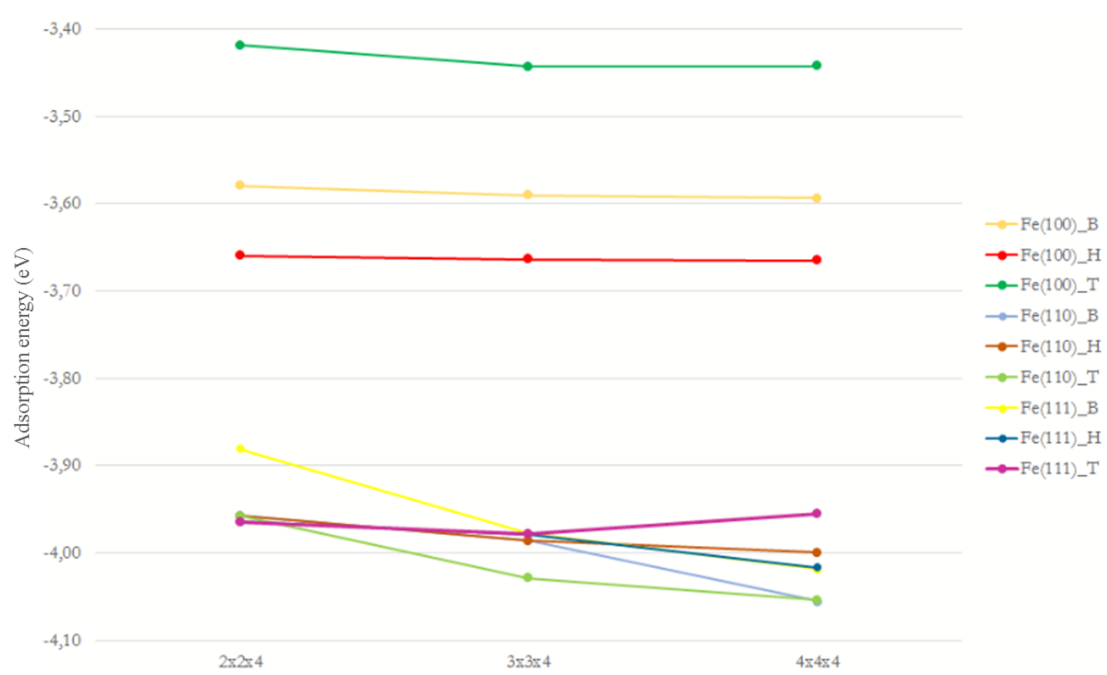


(b)



(c)

Figure 2. The adsorption energy against the number of layer of Al with cell area (a) 2x2, (b) 3x3, and (c) 4x4.



(a)

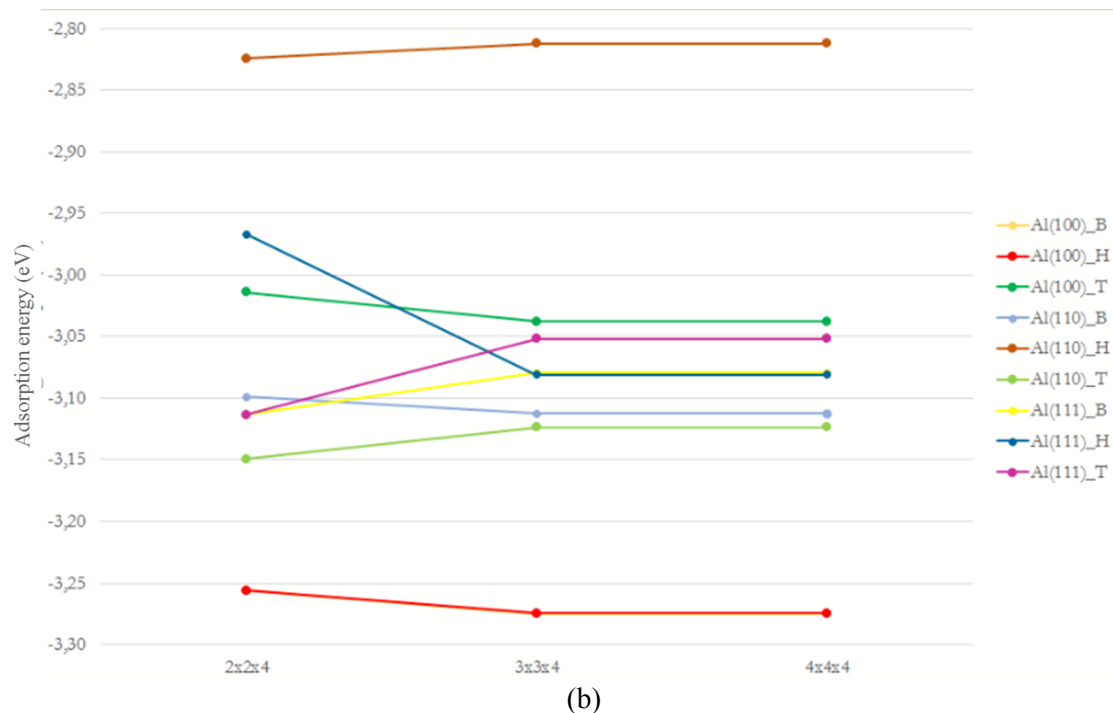


Figure 3. The adsorption energy against the cell area of (a) Fe and (b) Al.

### 3.2. The effect of increasing the cell area

Figure 3 shows the effect of increasing cell area on the adsorption energy of Fe and Al. The changes in adsorption energy are insignificant on both surfaces. The insignificant changes also indicated by the energy change is less than 0.1 eV. It occurs because of the number of atoms contribute in the system is many, while the obtained adsorption energy is small. Thus the energy is not enough to influence the vibrational movement in the system.

Based on Figure 3, increasing the cell area do not affect the adsorption energy. Thus, it is enough to use the minimum cell area in studying the hydrogen adsorption in Fe and Al surface.

## 4. Conclusion

Based on the analysis, we report that four layers is enough to study hydrogen adsorption on Fe and Al surface. The selection of the cell area is not necessarily considered.

## References

- [1] AG Saputro, MK Agusta, B Yuliarto, HK Dipojono, F Rusydi, R Maezono. Selectivity of CO and NO adsorption on ZnO (0002) surfaces: A DFT investigation. *Applied Surface Science*. 410 (2017), pp. 373–382.
- [2] Charles Kittel. *Introduction to Solid State Physics*. 8th Edition. John Wiley-Sons, 2005.
- [3] Peter Ferrin, Shampa Kandoi, Anand Udaykumar Nikelar, and Manos Mavrikakis. “Hydrogen adsorption, absorption, and diffusion on and in transition metal surface: A DFT study”. In: *Surface Science* 606 (2012), pp. 679–689.
- [4] David S. Sholl and Janice A. Steckel. *Density functional theory : a practical introduction*. Wiley, 2009. isbn: 978 0 470 37317 0.
- [5] P Giannozzi et al. “Advanced capabilities for materials modelling with Quantum ESPRESSO”. In: *Journal of Physics: Condensed Matter* 29.46 (2017), p. 465901.
- [6] Axel Gross. *Theoretical Surface Science. A Microscopic Perspective*. 2nd Edition. Springer-Verlag, 2007. isbn: 978-3-540-68966-9.