Density Functional Theory Study of Hydrogen Electroadsorption on the Pt(110) surfaces

Tran Thi Thu Hanh

Abstract — **The hydrogen adsorption on the Pt(110) and Pt(110)-(1x2) electrode surfaces has been investigated. To gain insight into detailed atomistic picture on the equilibrium coverage and structure, we have constructed a lattice gas model by determining the on-site energy and the interaction parameters using the first principles total-energy calculation. Therein atop, fcc, short bridge, long bridge and R, T, F, F' sites for H/Pt(110) and H/Pt(110)-(1x2) are covered by hydrogen atoms under various coverage conditions 0 ML < θ < 1 ML and the total-energy calculations are done for the (1x1) and (1x2) cells. The surface of (1×2) and (1×1) lateral unit cells. The convergence property with respect to the number of Pt layers and the k-point mesh are found. The comparison between different surface types are done. By comparing the calculated results with two different theoretical simulated data, SIESTA and VASP, we found good agreement between them.**

Index Terms—**hydrogen electroadsorption, platinum surface, density functional calculation.**

1 INTRODUCTION

Nowadays, electrochemical surface science has become an important tool in a number of diverse fields such as microelectronics, catalysis, and fuel cells [1,2]. Because of these applications, many studies focused on the adsorption on the metal surface. Among them, the hydrogen adsorptions on Pt(111), Pt(110) and Pt(100) surfaces have been paid special attention either under the ultra-high vacuum (UHV) [2,3], or in contact with the solution [1, 4-11].

Earlier, the UHV surface was theoretically investigated [12-20], and more recent studies [21-23] modeled the electrochemical interfaces with the UHV surface neglecting the hydration effect. As a tool to investigate the surfaces in UHV, the first-principles calculation has shown great success [24].

Among others, Pt(111) is the simplest surface where calculation can be done most accurately. In doing the theoretical calculation of H/Pt(111), it is worth mentioning that many forgoing calculation [12-19, 21-23] did not lead to the same conclusion regarding the most stable adsorption site. Some studies showed that the top site is the most stable site [12, 15, 18], while others found that the fcc is more stable than the top [19, 23]. This happened despite the fact that those calculations commonly used the density functional theory (DFT) within the generalized gradient approximation (GGA) for the exchange-correlation energy. This is due to insufficient parameters for the DFT-GGA calculation, in particular, insufficient number of k-points in the Brillouine zone integration and insufficient number of Pt layers for the slab model. Our previous research for H/Pt(111) started from accurate determination of the H adsorption energy within DFT-GGA. The calculated effective H-H interaction, or the g-value, was compared in good agreement with experiment [24].

The comparison nevertheless provides important insight into the H-adsorption, which prompts further theoretical investigation. For the H/Pt(110), the modeling is more complex. For the face-centered cubic FCC(110) surfaces, the unreconstructed (1×1) phase and the reconstructed (1×2) phase with missing-row exist. The (1×1) unit cell contains one substrate atom on the outermost row, the second and third layer atoms are still fairly exposed [24]. The (1×2) unit cell contains four more or less exposed Pt atoms [25, 26]. In practical applications, the Pt catalyst is often finely dispersed in small particles embedded in a matrix and the active sites can be of various types, such as, edges where crystal facets meet. The missing row reconstructed Pt(110)-(1×2) surface is a convenient

model for the edge sites formed between the most stable facets, or Pt(111). This fact motivated almost all theoretical calculations to use the missing row Pt(110)-(1×2) [25-29], reproducing thereby reasonable properties of the most stable adsorption site. Besides, the interaction of hydrogen with the Pt(110)-(1x1) surface has been also studied extensively both experimentally and theoretically [24, 25, 29, 30, 31].

However, up to now, there is still considerable disagreement as to the chemisorption site of H on Pt(110). The usual assumption of highly coordinated hydrogen [32, 33] sitting in the deep troughs of the missing rows was supported by work function measurements [24, 31] and vibrational spectroscopy [34], but was challenged by the first direct structure-probing experiment (Helium atom scattering, HAS), which led to the proposal of a highly coordinated subsurface site [35].

Besides, to study the adsorption of H on the missing row Pt(110)-(1×2), Engstrom et al. [24] and Shern [31] carried out low-energy electron diffraction (LEED), temperature-programmed desorption (TPD) and the mirror electron microscope LEED – that can measure the work function change. They supported the usual assumption [17, 18, 24] of highly coordinated H sitting in the deep troughs of the missing rows. Stenzel et al. [34] also supported the result using the vibrational spectroscopy measurement. However, Kirsten et al. [35] gave another proposal of a highly coordinated subsurface site on the basis of a direct structure-probing experiment (Helium atom scattering, HAS). On the contrary, Zhang et al. [29] performed LEED experiments and DFT calculations to provide an evidence that β_2-H is chemisorbed at the low coordinated short bridge site on top of the outermost Pt rows. Subsequently, Minca et al. [25] used TPD, quantitative LEED, and DFT to find a chemisorption site, called β_2-state, on the outermost close-packed rows under the ideal coverage of 0.5 ML. Adsorption sites on the (111) microfacets, called β_1-state, are occupied only at higher coverage. Note that the β_1 and β_2 states had been well described in Refs. [24, 30, 36]. Most recently, Gudmundsdóttir et al. [28] used TPD measurements and DFT calculations to confirm that, at low coverage, the strongest binding sites are the low coordination bridge sites at the edge. At higher coverage, on the other hand, H is adsorbed on higher coordination sites either on the micro-facet or in the trough. Those various foregoing researches had motivated us to carefully study the H chemisorption sites. To proceed this study, it will be important to investigate the chemisorption site more thoroughly, including the typical and atypical sites. The first purpose of the present work is to determine the binding sites and obtain the converged DFT data. We then compute the adsorption isotherm for Pt(110)-(1×2) using two different simulation software, the SIESTA and the VASP, and compare their results with those obtained for Pt(110)-(1x1) surface. Our study nevertheless provides important insight into the H-adsorption, which prompts further theoretical investigation.

2 COMPUTATIONAL METHODS

We used SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) package simulation. The linear combination of atomic orbitals (LCAO) and pseudopotential scheme implemented in SIESTA [25, 26] for the first-principle electronic structure calculations. Then the plane wave and projector augmented wave (PAW) potentials [27, 28] scheme implemented in VASP (Vienna Ab initio Software Package) [29, 30, 31] were used to supplement the SIESTA result. Fig. 1 shows the models and adsorption sites of the DFT calculation used for the calculation.
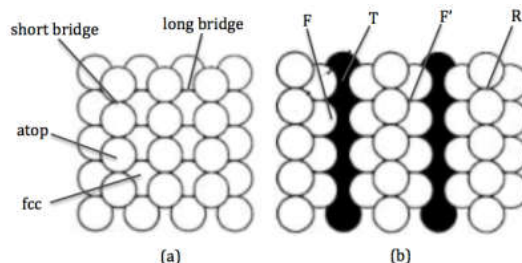

Figure 1. The (a)-Pt(110)-(1x1) and (b)-Pt(110)-(1×2) models were used for the DFT calculations. The surface was modeled using the repeated slab model. In the DFT calculation, the (1x1) and (1×2) lateral unit cells were used to construct the Pt(110)-(1×1) and Pt(110)-(1×2) slabs, corresponding. On Pt(110)-(1x1) surface, H atoms were adsorbed on the following sites; atop, long bridge, short bridge and fcc sites; on Pt(110)-(1x2) surface, H atoms were adsorbed on the following sites: the short bridge on the ridge (R), the on-top on the micro facet (F), the HCP hollow site (F') and the long bridge site in the trough (T).

We used the generalized gradient approximation (GGA) to the exchange-correlation functional due to Perdew, Burke, and Ernzerhof (PBE) for the DFT calculation [32]. The surface irreducible Brillouin zone was sampled on the k-point mesh generated by the Monkhorst-Pack (MP) scheme [33]. We used the repeated slab model to model the surface. The surface slab was separated from its periodic image by 16.6 Å, by which the interaction energy with the image can be reduced to 1 meV.

2.1 SIESTA calculation

We have adopted the following computational parameters for the SIESTA calculation. We used the double-zeta polarized (DZP) basic set, the mesh-cutoff of 200Ry. We employed the Fermi Dirac function with the electronic temperature of 300 K in carrying out the Brillouin zone integrations. We used the 200 meV value for the energy shift for the Pt, which determines the cutoff radius per angular momentum channel. For adsorbed H atoms, more extended basis is used in which we used the 60 meV value for the energy shift, and split norm of 0.53 for the second zeta. This ensures for us to obtain correct bond length and energy of H_2 molecule in which is important for the long-range interactions [9]. These standard computational parameters used in the SIESTA calculation had provided a reasonably accuracy both in the calculation of a bare Pt surface and a H_2 molecule [9]. The optimized lattice constant of 3.93 Å, which is in good agreement with the experimental bulk value of 3.924 Å [34] were used to construct the slabs.

The calculation of the H adsorbing surfaces was done for the following two sets of configurations. First, one H atom was adsorbed on the missing row Pt(110)-(1×2) surface of (1×2) lateral unit cell and on the Pt(110)-(1x1) surface of (1×1) lateral unit cell (Fig. 1). A vacuum equivalent to a twelve-layer slab separated the Pt slabs where the interlayer spacing was taken as 1.387 Å. The total energy was obtained after relaxing all the H and the Pt atoms of the upper four Pt-layers. This calculation was done mainly for the sake of comparing with previous calculations regarding the stability of the binding sites. Second, the surface of (1×2) and (1×1) lateral unit cells were used to investigate the convergence property with respect to the number of Pt layers and the k-point mesh. We used the spin-polarization calculations for all of the systems. In the Brillouin zone integration, 84 special k-points were used to sample the (12×12×1) MP grids for the (1×2) and (1×1) lateral unit cells.

2.2 VASP calculation

The VASP calculation was similarly done for two above sets of H-Pt configurations. Besides, we have used the k-point mesh ranging from (7×7×1) to (24×24×1) MP grids for the (1×2) lateral unit cell of H/Pt(110)-(1×2) system. And the number of Pt layers has changed from 5 to 19 layers when (12×12×1) MP grid was used for H/Pt(110)-(1x1) system. We have used the following computational parameters too. The plane wave cutoff energy was 400 eV, which is large enough to converge the total energy within the order of 1 meV per atom. The

Brillouin zone integrations were carried out by employing the Gaussian smearing function with the width 0.02 eV. The optimized lattice constant of the bare missing row Pt(110)-(1×2) and the Pt(110)-(1x1) obtained from the VASP calculation is 3.92 Å.

3 DFT DESCRIPTION OF H ON THE PT SURFACES

Previous calculations showed that the energy associated with the various binding sites on the surface is strongly dependent on the Θ_H. By adding the H-atoms to the surface one at a time, the surface is filled first at the strongest binding sites and finally at the weakest ones [24]. In this context, we first tested the order of the adsorption sites where they get filled by calculating the hydrogen adsorption energy

$$E_{ads} = E_{tot}(N_H) - E_{tot}(0) - \frac{n_H}{2}E_{H_2},$$

where $E_{tot}(N_H)$ is the total energy of the Pt surface adsorbed with N_H H atoms and E_{H2} is the total energy of the isolated H_2 molecule.

3.1 H/Pt(110)-(1x2)

For H/Pt(110)-(1x2) system, E_{ads} shows that the short bridge site on the ridge (R) is the strongest adsorption site, then the on-top on the micro facet (F), the HCP hollow site (F') and finally the long bridge site in the trough (T) (see Table 1). This result is in agreement with the results of Zhang et al. [18] and Gudmundsdóttir et al. [24]. Besides, Gudmundsdóttir et al. has shown that when the ridge has been filled, the preferred sites are the tilted on-top sites on the micro facets (F) followed by adsorption onto the long bridge sites in the trough (T). The filling of the trough sites forces the neighboring H-atoms to move from the on-top sites towards the HCP threefold hollow sites on the (111) micro facet (F').

TABLE 1. THE ADSORPTION ENERGY OF H ON PT(110)-(1X2) (EV). THE RESULTS FROM VASP CALCULATION ARE PARENTHESIZED.

cell	Pt layers	R	F	F'	T
		1/3 ML			
(1×2)	5	−0.649	−0.605	−0.564	−0.545
	7	−0.666	−0.632	−0.507	−0.497
	9	−0.737	−0.621	−0.497	−0.445
		(−0.555)	(−0.428)	(−0.343)	(−0.270)

Secondly, we calculated the optimized Pt-H bond lengths for the H on the Pt(110)-(1×2) as shown in Table 2.

TABLE 2. THE OPTIMIZED PT-H BOND LENGTH FOR
H/PT(110)-(1X2) (Å). THE RESULTS FROM VASP CALCULATION
ARE PARENTHESIZED.

cell	Pt layers	R	F	F'	T
		1/3 ML			
(1×2)	5	3.9	2.9	3.0	2.5
		(3.8)	(3.0)		
	7	3.9	2.9	2.9	2.4
		(3.8)	(3.0)		
	9	3.9	2.9	2.8	2.4
		(3.8)	(2.9)	(2.8)	(2.6)

We have confirmed that the results were affected by less than 1% when changing the number of Pt layers from five to nine. To obtain the converged value, we now investigate in detail the convergence property with respect to the number of Pt layers and k-points.

TABLE 3: THE ADSORPTION ENERGY OF H ON PT(110)-(1X2)
(EV), USING (12×12×1) MP GRID FOR SIESTA AND VASP
CALCULATIONS.

Pt layers	SIESTA		VASP	
	R	F	R	F
5	-0.649	-0.605	-0.483	-0.420
6	-0.770	-0.579	-0.597	-0.311
7	-0.666	-0.631	-0.492	-0.440
8	-0.715	-0.594	-0.537	-0.398
9	-0.737	-0.621	-0.555	-0.428
10	-0.683	-0.614	-0.507	-0.422
11	-0.743	-0.598	-0.562	-0.407
12	-0.703	-0.619	-0.523	-0.423
13	-0.718	-0.608	-0.542	-0.417
14	-0.735	-0.615	-0.551	-0.422
15			-0.521	-0.426
16			-0.553	-0.415
17			-0.534	-0.425
18			-0.535	-0.418
19			-0.550	-0.425

Previous calculation for Pt(111) provided the dependence of the adsorption energy on k-point mesh and number of Pt layers [9]. Therefore, in this work, the calculation was done similarly using (1×2) lateral unit cell, on which one H atom was let adsorb either on the R or on the F. Table 3 shows the calculated adsorption energy and Fig.2 plots the adsorption energy on the F relative to that on the R, E_{ads}.
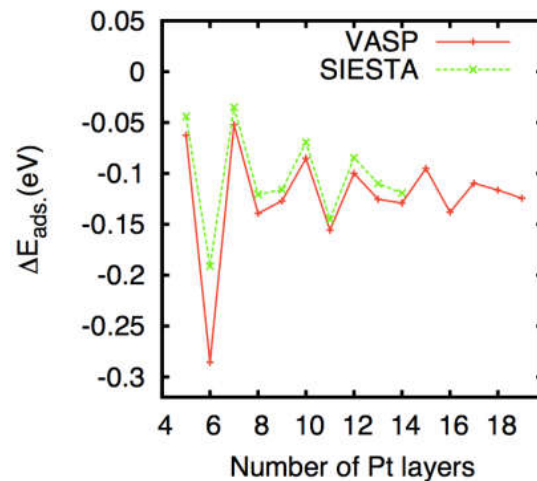

Figure 2. The relative adsorption energy, $E_{ads}(R)$ $E_{ads}(F)$ for H/Pt(110)-(1x2), calculated using SIESTA and VASP calculation.

The table shows that the SIESTA calculation provides the adsorption energy systematically larger by 0.15 eV in magnitude, while the figure shows that they provide a similar dependence on the number of Pt layers as it changes from 5 to 19 layers when (12×12×1) MP grid was used. From the Fig. 2 we found that for the low Pt layers (less than 9), the value oscillates with large amplitude, then the oscillation is regular and periodic when taking 9 to 19 layers. It suggests that the converged value has already been determined well around 0.12 eV within the amplitude of the oscillation (□ 40 meV) by taking these layers.
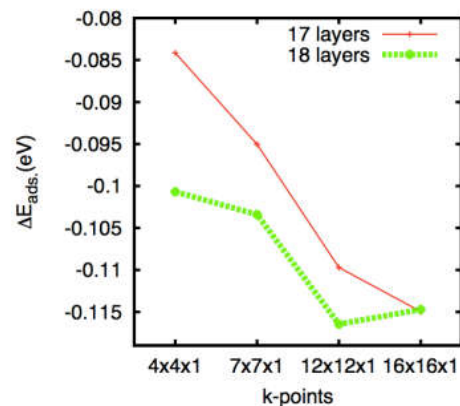

Figure 3. k-point dependence of E_{ads}.

Fig. 3 plots the dependence on k-points, which shows that the results for various number of Pt layers becomes very close to each other when using (16×16×1) MP grid. From these results we conclude that the converged E_{ads} is located at around 0.12 eV. It means that the R obviously is more stable than F by that amount. This is our conclusion on the theoretical adsorption energy within the UHV surface and DFT-PBE for H/Pt(110)-(1x2) system.

3.2 H/Pt(110)

Similar calculation of E_{ads} for H/Pt(110)-(1x2) system shows that the short bridge site is the strongest adsorption site, then the on-top site, the long bridge site and finally the fcc site (see Table 4).

TABLE 4. THE ADSORPTION ENERGY OF H ON PT(110)-(1x1) (EV), USING SIESTA CALCULATION.

cell	Pt layers	short bridge	top	long bridge
		1 ML		
(1x1)	3	-0.915	-0.942	-0.323
	4	-0.798	-0.693	
	5	-0.782	-0.692	-0.279
	6	-0.835	-0.768	
	7	-0.770	-0.642	
	8	-0.815	-0.739	
	9	-0.807	-0.688	

From the calculation data, the short bridge site (B) and the on-top site (OT) are the most stable sites on the surface. Therefore, in the next step, we calculated the optimized Pt-H bond lengths only for the B and OT sites of H on the Pt(110)-(1×2) (as shown in Table 5).

TABLE 5. THE OPTIMIZED PT-H BOND LENGTH FOR H/Pt(110)-(1x1) (Å), USING SIESTA CALCULATION.

cell	Pt layers	short bridge	top
		1 ML	
(1x1)	5	1.78	1.58
	7	1.78	1.57
	9	1.78	1.57

We have also confirmed that the results were affected by less than 1% when changing the number of Pt layers from five to nine. Besides, base on the successful calculation for the converged value of H/Pt(110)-(1x2) system, we now similarly investigate the convergence property with respect to the number of Pt layers and k-points for H/Pt(110)-(1x1) system. The calculation was done similarly using (1x1) lateral unit cell, on which one H atom was let adsorb either on the B or on the OT. The Fig.4 plots the adsorption energy on the OT site relative to that on the B site, ΔE_{ads}, when the number of Pt layers was changed from 5 to 18 layers and (12×12×1) MP grid was used. From the Fig. 4 we found that for the low Pt layers (less than 10), the value oscillates with large amplitude, then the oscillation is regular and periodic when taking 10 to 18 layers. It suggests that the converged value has already been determined well around −0.11 eV within the amplitude of the oscillation ($\square$ 50 meV) by taking these layers. From these results we conclude that the converged ΔE_{ads} is located at around −0.11 eV. It means that the B obviously is more stable than OT by that amount.
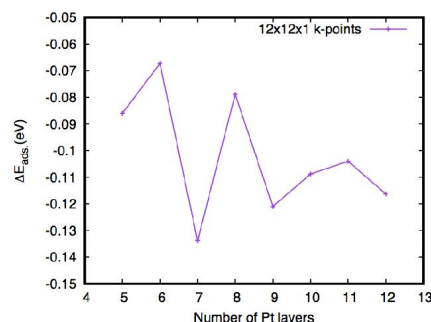

Figure 4. Pt layer dependence of the relative adsorption energy, E_{ads}(short bridge)−E_{ads}(top) for H/Pt(110)-(1x1), calculated using VASP calculation.

4 CONCLUSIONS

A converged first-principles DFT-GGA was used to investigate the hydrogen adsorption on the Pt(110) surfaces. It was shown that: for the H/Pt(110)-(1x2) system, the short bridge site on the ridge (R) is the strongest adsorption site, then the on-top on the micro facet (F), the HCP hollow site (F') and finally the long bridge site in the trough (T). The result is in consistent with the LEED experimental and the DFT theoretical results found in the literature. Besides, for the H/Pt(110)-(1x1) system, it was also shown that, the short bridge site is the strongest adsorption site, then the on-top site, the long bridge site and finally the fcc site. These determined sites are playing an important role to study the nature of H adsorbed on Pt surfaces, such as the interaction between hydrogen on the surface, and compare them with experimental data. Therefore, further investigation of the effective H-H interaction on the Pt(110) surfaces is required to compare the theoretical and experimental isotherm.

REFERENCES

[1]   N. M. Markovíc, B. N. Grgur, and P. N. Ross, J. Phys. Chem. B 101 (1997) 5405.

[2]   K. Christmann, G. Ertl and T. Pignet, Surf. Sci. 54 (1976) 365.

[3]   P. Nordlander, S. Holloway, J.K. Nørskov, Surf. Sci. 136, (1984) 59.

[4]   H. Kita, J. Mol. Catal. A: Chem. 199 (2003) 161.

[5]   K. Kunimatsu, T. Senzaki, G. Samjeske, M. Tsushima, and M. Osawa, Electrochim. Acta 52 (2007) 5715.

[6]   G. Jerkiewicz, Prog. Surf. Sci. 57 (1998) 137.

[7]   A. Zolfaghari, G. Jerkiewicz, J. Electroanal. Chem. 467 (1999) 177.

[8]   N. M. Marković, T. J. Schmidt, B. N. Grgur, H. A. Gasteiger, R. J. Behm, P. N. Ross, J. Phys. Chem. B 103 (1999) 8568.

[9]   N. M. Marković and P. N. Ross, Surf. Sci. Rep. 45 (2002) 117.

[10] J. Clavilier, A. Rodes, K. Elachi, and M.A. Zamakhchari, J.

de Chim. Phys. et de Physico-Chemie Biol. 7-8 (1991) 1291.

[11] B.E. Conway, G. Jerkiewicz, Electrochim. Acta 45 (2000) 4075.

[12] X. Zhang and H. Xiang, International Journal of Heat and Mass Transfer 84 (2015) 729.

[13] B. Dai, B. Zheng and L. Wang, Applied Mathematics and Computation 219 (2013) 10044.

[14] G.W. Watson, R.P.K. Wells, D.J. Willock, G. J. Hutchings, Phys. Chem. B 105 (2001) 4889.

[15] S. C. Bădescu, P. Salo, T. Ala-Nissila, S. C. Ying, Phys. Rev. Lett. 88 (2002) 136101.

[16] S. C. Bădescu, K. Jacobi, Y. Wang, K. Bedurftig, G. Ertl, P. Salo, T. Ala- Nissila and S. C. Ying, Phys. Rev. B 68 (2003) 205401.

[17] P. Legare, J. Surf. Sci. 599 (2004) 169.

[18] D. C. Ford, Y. Xu, M. Mavrikakis, J. Surf. Sci. 587 (2005) 159.

[19] J. Greeley, M. Mavrikakis, J. Phys. Chem. B 109 (2005) 3460.

[20] B. Hammer, J. K. Nørskov, Nature 376 (1995) 238.

[21] G. S. Karlberg, T. F. Jaramillo, E. Skúason, J. Rossmeisl, T. Bligaard, and J. K. Nøskov, Phys. Rev. Lett. 99 (2007) 126101.

[22] E. Skúason, G. S. Karlberg, J. Rossmeisl, T. Bligaard, J. Greeley, H. Jónsson, J. K. Nøskov, Phys. Chem. Chem. Phys. 9 (2007) 3247.

[23] I. Hamada, Y. Morikawa, J. Phys. Chem. C 112 (2008) 10889.

[24] T.T.T. Hanh, Y. Takimoto, O. Sugino, Surf. Sci. 625 (2014) 104.

[25] J.R. Engstrom, W. Tsai, and W.H. Wweinberg, J. Chem. Phys. 87 (1987) 3104.

[26] M. Minca, S. Penner, T. Loerting, A. Menzel, E. Bertel, R. Zucca, and J. Redinger, Topics in Catalysis 46 (2007) 161.

[27] S. Gudmundsdóttir, E. Skúlason, and H. Jónsson, Phys. Rev. Lett. 108 (2012) 156101.

[28] S. Gudmundsdóttir, E. Skúlason, K.J. Weststrate, L. Juurlink, and H. Jónsson, Phys. Chem. Chem. Phys. 15 (2013) 6323.

[29] Z. Zhang, M. Minca, C. Deisl, T. Loerting, A. Menzel, E. Bertel, Phys. Rev. B 70 (2004) 121401.

[30] G. Anger, H. F. Berger, M. Luger, S. Feistritzer, A. Winkler and K. D. Rendulic, Surf. Sci. 219 (1989) L583.

[31] C. S. Shern, Surf. Sci. 264 (1992) 171.

[32] G. Burns, Solid State Physics (Academic, New York, 1985).

[33] K. Christmann, Surf. Sci. Rep. 9 (1988) 1.

[34] W. Stenzel, S. Jahnke, Y. Song, and H. Conrad, Prog. Surf. Sci. 35 (1991) 159.

[35] E. Kirsten, G. Parschau, W. Stocker, and K. Rieder, Surf. Sci. 231 (1990) L183.

[36] C. Lu and R. I. Masel, J. Phys. Chem. B 105 (2001) 9793.

Tran Thi Thu Hanh is with the Computational Physics Lab., the Faculty of Applied Science, Ho Chi Minh City University of Technology, VNU-HCM, 268 Ly Thuong Kiet st., Dist. 10, Ho Chi Minh City, Viet Nam (e-mail: thuhanhsp@hcmut.edu.vn).

Nghiên cứu lý thuyết phím hàm mật độ về sự hút bám điện tử của hydro trên các dạng bề mặt Pt(110)

Trần Thị Thu Hạnh

Tóm tắt - **Sự hấp thụ của hydro trên bề mặt điện cực Pt(110) và Pt (110)-(1×2) khuyết dãy được tiến hành nghiên cứu. Để có được cái nhìn sâu sắc về bức tranh nguyên tử về độ bao phủ và cấu trúc cân bằng, chúng tôi đã xây dựng một mô hình khí lưới bằng cách xác định năng lượng vị trí và các thông số tương tác thông qua việc sử dụng cách tính tổng năng lượng theo nguyên lý ban đầu. Trong đó các vị trí trên đỉnh, fcc, cầu ngắn, cầu dài và các vị trí R, T, F, F' cho hệ H/Pt(110) và H/Pt(110)-(1x2) được bao phủ bởi các nguyên tử hydro theo các điều kiện bao phủ khác nhau 0 ML < θ < 1 ML và tính toán tổng năng lượng được thực hiện cho các ô đơn vị mạng (1x1) và (1x2). Thuộc tính hội tụ đối với số lớp Pt và điểm k được tính toán. Việc so sánh kết quả tính toán giữa các loại bề mặt khác nhau được thực hiện. Bằng cách so sánh các kết quả tính toán với hai dữ liệu mô phỏng lý thuyết khác nhau, SIESTA và VASP, chúng tôi đã tìm thấy kết quả tốt phù hợp giữa hai phương pháp này.**

Từ khóa - **hấp thụ điện tử hydro, bề mặt platin, tính toán phiếm hàm mật độ.**