

Research Article

The Adsorption and Diffusion Manners of Hydrogen Atoms on Pt (100), Pt (110), and Pt (111) Surfaces

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In this study, the interactions between H atoms and the (100), (110), and (111) surfaces of platinum have been investigated by using the London-Eyring-Polanyi-Sato (LEPS) potential function. The adsorption zones (sites) and LEPS energy values of these sites have been determined theoretically. In addition, the potential-energy surfaces for each Pt surface have been obtained in detail. Further, the adsorption sites on the surface, scattering from the surface, diffusion paths on the surface, and transition regions to the subsurface, have been determined and the differences have been examined in detail among the surfaces. From these results, it is found that an H atom has the lowest binding energy at the hollow sites on the Pt (100) and Pt (111) surfaces and that it has the lowest binding energy at the long-bridge sites on the Pt (110) surface. It has also been determined that the hollow sites on the three surfaces are the regions through which H atoms can penetrate into the subsurface. In addition, it has also been found that, for each of the three Pt surfaces, the diffusion of an H atom across the surface may follow a bridge-hollow-bridge pathway. These results are in agreement with previous experimental and theoretical results. Besides, the adsorption and diffusion manners of hydrogen atoms on each of the Pt surfaces have been analyzed deeply.

1. Introduction

The results of research on the interaction of hydrogen atoms and transition-metal surfaces have helped a large number of technological studies such as material fragility, hydrogen fuel cell, hydrogen storage, and catalytic corrosion control. For this purpose, experimental [1–7] and theoretical [2–4, 8–28] investigations were carried out on the platinum surface and hydrogen interaction. (111), (110), and (100) surfaces of platinum were used in these studies. Through these studies it has been observed that the different faces of the metal surface show different properties.

Hydrogen adsorption on the (100), (110), and (111) surfaces of platinum has been studied experimentally both by voltammetry and by *in situ* infrared reflection and absorption spectroscopy [1]. The results show that these surface crystallographic orientations are sensitive areas for hydrogen adsorption [1]. Based on these experimental studies, atomic and molecular hydrogen interactions with a Pt (111) surface

have been studied theoretically using the density-functional-theory (DFT) method [8]. The results indicate that there is no—or a very low—energy barrier for H₂ dissociation. However, the preferential adsorption sites for hydrogen atoms on the Pt surface could not be determined in this investigation [8].

Zhang et al. [2] have used both quantitative low-energy electron diffraction (LEED) and DFT calculations to investigate experimentally and theoretically the growth of one-dimensional adsorbate structures, using hydrogen-modified Pt (110) as a model. In a similar study, Minca et al. [3] investigated experimentally and theoretically the chemisorption of hydrogen on a missing-row, reconstructed Pt (110)-(1x2) surface by using temperature-programmed desorption (TPD), quantitative LEED, and DFT calculations. According to these results, the short-bridge site was found to be the most favorable for hydrogen adsorption on a Pt (110) surface [2, 3]. In addition, Gudmundsdóttir et al. [4] have performed TPD measurements and DFT calculations to study experimentally

and theoretically the adsorption of hydrogen atoms on a Pt (110)-(1x2) surface. They reported also that low-coordination bridge sites are preferential adsorption sites for hydrogen atoms on the surface [4].

Qiaocui Shi and Rong Sun [9] have used DFT calculations to investigate the adsorption of hydrogen on the Pt (100), Pt (110), and Pt (111) surfaces with different surface coverages. According to their results [9], the 3-fold, fcc-hollow site is suitable for the adsorption of H on Pt (111), while the bridge sites are favored for the Pt (100) and Pt (110) surfaces. In addition, Vasic et al. [10] employed a DFT calculation with a generalized gradient approximation (DFT-GGA) to study the dissociative adsorption of hydrogen on Pt (111), Pt (100), and Pt (110) in the range of coverage from 0.25 to 1 monolayer. They found that the fcc-hollow site is the preferential adsorption site for Pt (111), while the bridge and short-bridge sites are suitable for the adsorption of hydrogen on the Pt (100) and Pt (110) surfaces, respectively [10]. Another theoretical study [11] reported the same adsorption sites for these three Pt surfaces.

Ferrin et al. [12] have employed periodic, self-consistent DFT-GGA (PW91) calculations to analyze hydrogen adsorption, absorption, and diffusion on and in transition-metal surfaces, including the Pt (100) and (111) surfaces. They reported that the fcc-hollow sites and bridge sites are the most convenient adsorption sites for hydrogen atoms on the Pt (100) and (111) surfaces, respectively [12]. Denise C. Ford et al. [13] utilized self-consistent, periodic, density-functional theory (DFT-GGA) calculations to study theoretically atomic and molecular adsorption on Pt (111). They used both the GGA-PW91 and the RPBE methods for their calculations. According to both results, H atoms were found to have very similar binding-energy values at the top, bridge, fcc-hollow, and hcp-hollow regions of the Pt (111) surface [13].

Another theoretical study [14] calculated the adsorption, vibration, and diffusion of H atoms on the Pt (100), (110), and (111) surfaces using a five-parameter Morse potential to define the interaction between an adatom and a metal-surface cluster. These studies obtained four major results: First, a 4-fold hollow site was found to be the only adsorption site on the Pt (100) surface. Second, the pseudo-3-fold hollow (H3) and long-bridge (LB) sites were the most stable sites at low coverage, while with increasing coverage, the H atoms were also adsorbed at the short-bridge (SB) sites on the Pt (110) surface. Last, the 3-fold hollow site was found suitable for the adsorption of H atoms on the Pt (111) surface [14]. Further, Graeme W. Watson et al. [15] used gradient-corrected DFT calculations to study theoretically the adsorption and thermally activated diffusion pathways of hydrogen on a Pt (111) surface. They also obtained the adsorption energies for the different adsorption sites [15].

In the present work, we have studied in detail the adsorption and diffusion of hydrogen atoms on Pt (100), Pt (110), and Pt (111) surfaces using the London-Eyring-Polanyi-Sato (LEPS) potential function. In the next section, we discuss the theoretical model and the LEPS potential. We present our results, provide discussion, and give our conclusions in subsequent sections.

2. Theoretical Method

2.1. The LEPS Function. The LEPS potential is a convenient potential-energy function for studies of adsorbate-surface interactions. This potential has been employed to investigate the interactions of one or two hydrogen atoms with nickel clusters [29]. In another investigation, the H/2H-Cu(111) interaction system was studied using the LEPS potential function, as described in detail in [30]. It is significant that the LEPS parameters, including the Morse parameters, have to be obtained separately for each new interaction system. We have determined these parameters in our previous study of the interaction of H with Pt (111) [16].

In the present study, we have used the same parameters to analyze the interactions of H with the Pt (100) and Pt (110) surfaces. The LEPS potential, which includes the Coulomb (Q) and exchange (J) functions, can be written in the form

$$\begin{aligned} V_{LEPS}(X_A, X_B, \{X_S\}) \\ = Q_{A,B} + Q_{A,S} + Q_{B,S} \\ - [J_{A,B}(J_{A,B} - J_{A,S} - J_{B,S}) + (J_{A,S} + J_{B,S})^2]^{1/2}. \end{aligned} \quad (1)$$

Here, A and B denote hydrogen atoms and S represents all the surface atoms. The quantities X_A , X_B , and $\{X_S\}$ are the positions of the hydrogen atoms and the surface atoms, respectively. The pairs of subscripts (A,S) and (B,S) designate the interactions between the hydrogen atoms and the surface atoms, while the subscripts (A,B) denote the interactions between the hydrogen atoms. The Coulomb functions $Q_{A,B}$ and $Q_{A,S}$ and the exchange functions $J_{A,B}$ and $J_{A,S}$ are given by

$$Q_{A,B} = \frac{D_e}{4(1 + \Delta_{A,B})} \left\{ (3 + \Delta_{A,B}) e^{-2\alpha_e(R-R_e)} \right. \quad (2)$$

$$\left. - (2 + 6\Delta_{A,B}) e^{-\alpha_e(R-R_e)} \right\}$$

$$Q_{A,S} = \frac{1}{4(1 + \Delta_{A,S})} \left\{ (3 + \Delta_{A,S}) \right. \quad (3)$$

$$\left. \cdot \left(D_H e^{-2\alpha_H(r_s - r_H)} + \sum_{K=1}^N D_2 e^{-2\alpha_2(R_{A,S} - r_2)} \right) \right.$$

$$\left. - (2 + 6\Delta_{A,S}) \right\}$$

$$\left. \cdot \left(D_H e^{-\alpha_H(r_s - r_H)} + \sum_{K=1}^N D_2 e^{-\alpha_2(R_{A,S} - r_2)} \right) \right\}$$

$$J_{A,B} = \frac{D_e}{4(1 + \Delta_{A,B})} \left\{ (1 + 3\Delta_{A,B}) e^{-2\alpha_e(R-R_e)} \right. \quad (4)$$

$$\left. - (6 + 2\Delta_{A,B}) e^{-\alpha_e(R-R_e)} \right\}$$

TABLE I: LEPS parameters for the H – Pt (100), (110), and (111) interaction systems.

| | | |
|-------------------------------------|-------------------------------------|---------------------------|
| $\Delta_{H,H} = 0.000$ | $D_2 = 0.148 \text{ eV}$ | $\Delta_{H,Pt} = 0.346$ |
| $D_e = 4.745 \text{ eV}$ | $D_H = 2.000 \text{ eV}$ | $R_H = 2.320 \text{ \AA}$ |
| $\alpha_e = 1.900 \text{ \AA}^{-1}$ | $\alpha_2 = 1.480 \text{ \AA}^{-1}$ | $R_2 = 2.010 \text{ \AA}$ |
| $R_e = 0.733 \text{ \AA}$ | $\alpha_H = 1.040 \text{ \AA}^{-1}$ | $N_{6s} = 0.670$ |

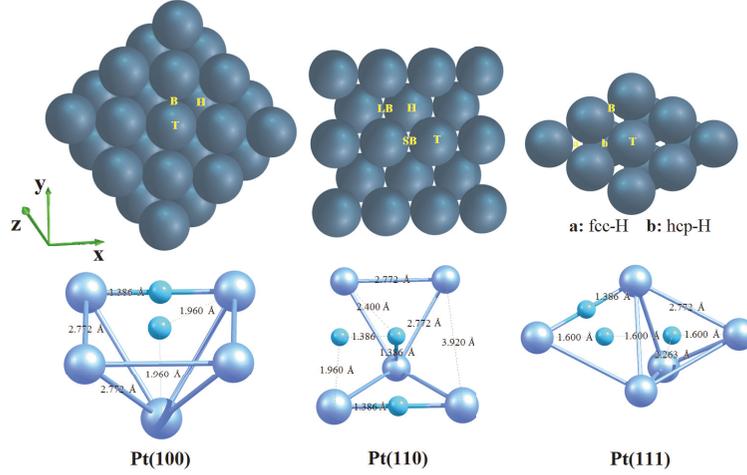


FIGURE 1: Top view of the highly symmetric sites on the Pt (100), Pt (110), and Pt (111) surfaces, together with the distances between the sites and the nearest surface atoms.

$$\begin{aligned}
 J_{A,S} = & \frac{1}{4(1 + \Delta_{A,S})} \left\{ (1 + 3\Delta_{A,S}) \right. \\
 & \cdot \left(D_H e^{-2\alpha_H(r_s - r_H)} + \sum_{K=1}^N D_2 e^{-2\alpha_2(R_{A,S} - r_2)} \right) \\
 & - (6 + 2\Delta_{A,S}) \\
 & \left. \cdot \left(D_H e^{-\alpha_H(r_s - r_H)} + \sum_{K=1}^N D_2 e^{-\alpha_2(R_{A,S} - r_2)} \right) \right\}.
 \end{aligned} \quad (5)$$

Here, $R = |X_A - X_B|$ and $R_{A,S} = |X_A - X_S|$. The other quantities in (2)–(5) are the LEPS parameters obtained in [16] and shown in Table 1.

2.2. Pt (100), (110), and (111) Surfaces. The Pt surfaces used in this study are arranged as a slab of six atomic layers in an ABCA ordering. In the face-centered cubic (fcc) surface structure, the Pt (100) and Pt (110) surfaces contain 663 Pt atoms, while the Pt (111) surface consists of 1092 Pt atoms. The ABC layers of the Pt (100) and Pt (110) surfaces contain 121, 100, and 121 Pt atoms, respectively. In addition, for the Pt (111) surface, 179, 178, and 189 Pt atoms, respectively, are located in the ABC layers. The lattice constant of Pt was taken to be 3.92 Å [31] to construct the surfaces, and the spaces between the layers are 1.960 Å, 1.386 Å, and 2.263 Å for the Pt (100), Pt

(110), and Pt (111) surfaces, respectively. Pt atoms of the slab were taken as fixed.

Highly symmetric sites on the surfaces shown in Figure 1 have been taken into account in calculating the potential energies of the interactions of H with the Pt (100), Pt (110), and Pt (111) surfaces. The Pt (100) surface has the following highly symmetric sites: a top (T), bridge (B), and hollow (H). The highly symmetric sites for the Pt (110) surface are a top (T), hollow (H), SB, and LB, while they are a top (T), bridge (B), hcp-hollow (hcp-H), and fcc-hollow (fcc-H)—i.e., with no underlying substrate atom located in the second layer—for the Pt (111) surface. The distances between the sites and the nearest surface atoms are also shown in Figure 1.

3. Results and Discussion

The binding energies of the H atoms and their heights above the surfaces that correspond to these energies are shown in Table 2 for each Pt surface and for all of the sites. The energies of the H atom for the top, hollow, and bridge sites of the Pt (100) surface are -2.28 , -2.83 , and -2.52 eV, respectively. For these sites, the heights of the H atoms are 1.55, 0.55, and 1.15 Å, respectively. Moreover, the binding energies of the H atom for the top, hollow, SB, and LB sites on the Pt (110) surface are -2.18 , -2.73 , -2.39 , and -2.84 eV, respectively. For these sites, the heights of the H atoms are 1.6, 0.4, 1.0, and 0.2 Å, respectively. Finally, the binding energies of the H atom for

TABLE 2: The energies E of H atoms on Pt surfaces at $z = 0.0 \text{ \AA}$, the equilibrium heights z , the binding energies E_b at these heights, and the heights z_1 of the H atom from the second-layer slab for each interaction system and for each highly symmetric site.

| Systems | Sites | E (eV) | z (\AA) | E_b (eV) | z_1 (\AA) |
|-------------|-------|-----------------------|----------------------|------------|------------------------|
| | | $z = 0.0 \text{ \AA}$ | | | |
| H - Pt(100) | T | ---- | 1.55 | -2.28 | 3.51 |
| | H | -2.66 | 0.55 | -2.83 | 2.51 |
| | B | 0.04 | 1.15 | -2.52 | 3.11 |
| H - Pt(110) | T | ---- | 1.60 | -2.18 | 2.99 |
| | H | -1.2 | 0.40 | -2.73 | 1.79 |
| | SB | 0.06 | 1.00 | -2.39 | 2.39 |
| | LB | -2.79 | 0.20 | -2.84 | 1.59 |
| H - Pt(111) | T | ---- | 1.60 | -2.31 | 2.99 |
| | fcc-H | -1.05 | 1.00 | -2.65 | 2.39 |
| | hcp-H | -1.12 | 1.00 | -2.64 | 2.39 |
| | B | 0.10 | 1.20 | -2.59 | 2.59 |

z_1 : Height of the H atom from the second-layer surface.

the top, fcc-hollow, hcp-hollow, and bridge sites on the Pt (111) surface are -2.31 , -2.65 , -2.64 , and -2.59 eV, respectively. For these sites, the heights of the H atoms are 1.6, 1.0, 1.0, and 1.2 \AA , respectively. Table 2 lists the energy E of an H atom on a Pt surface at $z = 0.0 \text{ \AA}$, the equilibrium heights z , the binding energies E_b at these heights, and the heights of the H atoms from the second-layer slab for each interaction system and for each highly symmetric site.

For the Pt (100), (110), and (111) surfaces, the LEPS energy curves as functions of the height of the H atom over the Pt surface are plotted in Figure 2, which compares them for all of the sites and each of the surfaces. Figure 3 shows column graph of the LEPS energy values for the highly symmetric sites of the Pt (111), (110), and (111) surfaces, grouped according to the different heights $z = -0.6, 0.0, 0.6, 1.0$, and 1.2 \AA . When an H atom is on the surface at a height of 0.0 \AA , the attractive potential due to the surface atoms is dominant for all of the hollow sites on the Pt (100), (110), and (111) surfaces and for the LB site on Pt (110), as indicated in Table 2 and Figures 2 and 3. This demonstrates that the hollow sites are more suitable for the adsorption of hydrogen atoms on the Pt (100) and Pt (111) surfaces, whereas the LB region is better for the Pt (110) surface, as indicated in Figures 2 and 3. The binding energy for the Pt (110) surface was found to be the lowest among the three surfaces. In addition, we note that an H atom adsorbed at the minimum binding energy at the LB site of the Pt (110) surface is at the position closest to the surface and to the second-layer surface, as compared to the Pt (100) and Pt (111) surfaces.

According to some studies, the hollow, LB, and fcc-hollow sites were found to be the adsorption regions for H atoms on Pt (100) [14], Pt (110) [14], and Pt (111) [9–12, 14, 17–22], respectively. Other studies have reported the bridge site, the SB site, and the top site as the adsorption sites for H atoms on Pt (100) [2–4, 9–12], Pt (110) [2–4, 9–11], and Pt (111) [13, 24–26], respectively. The results of these previous theoretical and experimental studies are shown in Table 3 for comparison with the results from the present study.

Hydrogen atoms can become trapped at different heights below the metal surface. These trapping zones can be seen in the contour plots of the calculated potential-energy surfaces shown in Figure 4. At 0.6 \AA depth, we find that the surfaces have H atom trapping features at the hollow sites. In contrast, at 1.2 \AA depth, we observed that the trapping region and the propagation route for the H atoms lie immediately below the locations of the first-layer surface atoms, due to the energy barriers originating from the second-layer surface atoms.

When an H atom is located exactly on the surface, it is also exposed to the repulsive surface potentials of the B and SB sites in addition to the top sites. As can be seen clearly in Figures 2 and 4, when an H atom is exactly on a Pt (100) or a Pt (111) surface, it is trapped at a hollow site, due to the repulsive potentials caused by the top and bridge sites. However, an H atom does not encounter any potential barrier along the H-LB-H pathway on a Pt (110) surface.

For the Pt (110) surface at $z = 0.0 \text{ \AA}$, Figure 4 shows clearly the effect of the attractive surface potential along the hollow-long-bridge-hollow sites. Along this route, an H atom is easily held on the surface, while at the same time it can propagate across the surface. Moreover, for the Pt (110) surface, an H atom can penetrate into the subsurface through the LB and hollow areas, while it can just penetrate *via* the hollow sites of the Pt (100) and Pt (111) surfaces. Figure 4 shows clearly that an H atom cannot penetrate into the subsurface from a bridge site or a SB site, due to the minor repulsive potentials of the surface atoms. Nevertheless, if an H atom impacts a B or SB site on the surface with sufficient kinetic energy, it can pass into the subsurface through these sites. In addition to being subsurface transition zones, these sites thus are also trapping zones for the H atoms, as shown in Figure 4.

Figure 5 shows contours of the potential-energy surfaces plotted for different heights of an H atom above the surface. At a height of 0.6 \AA , the bridge regions of the Pt (100) and Pt (111) surfaces—and the SB region for the Pt (110) surface—have approximately the same adsorption energy, while differences between the adsorption energies are clearly

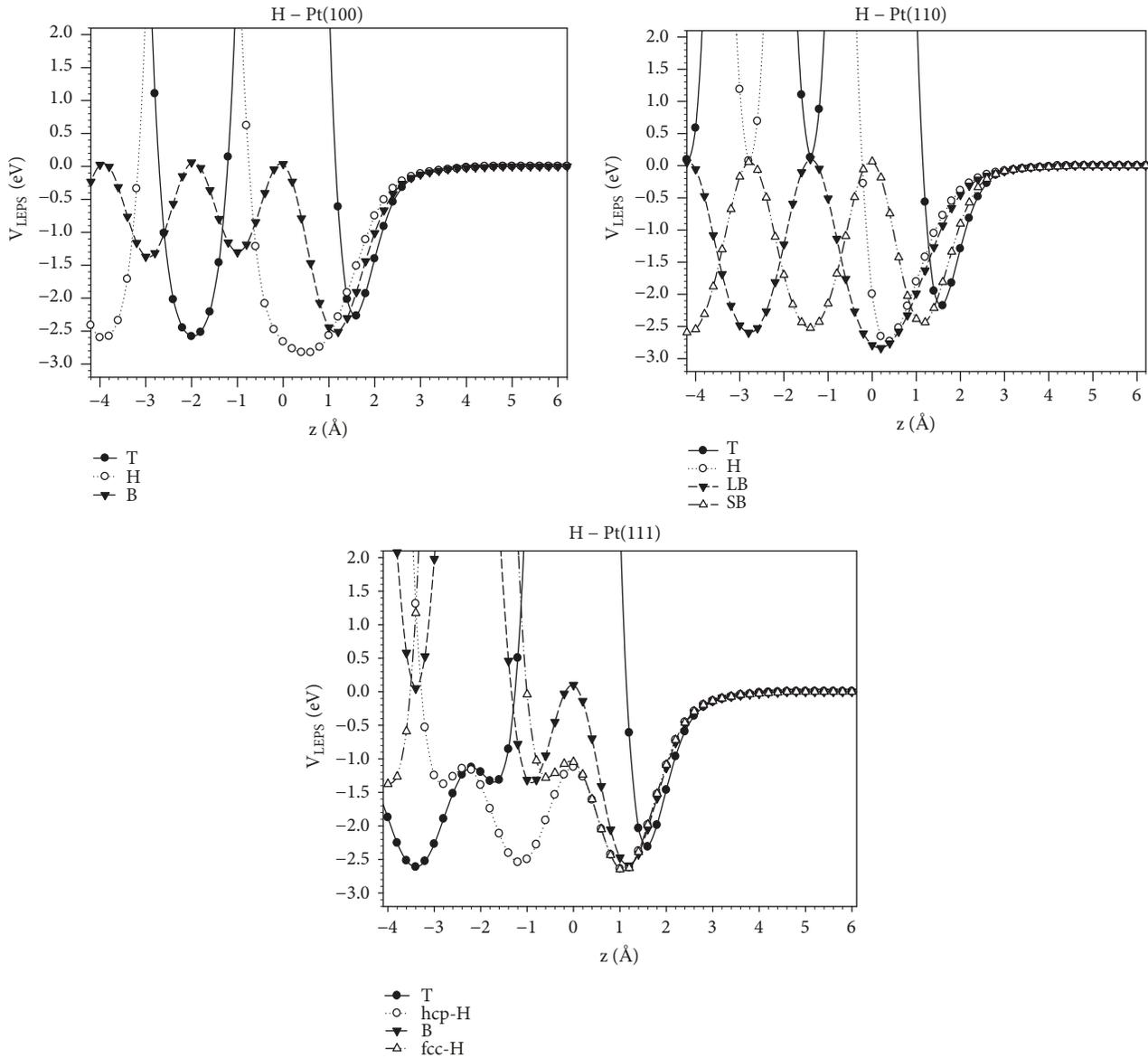


FIGURE 2: The LEPS potential-energy values plotted as functions of z [the height of an H atom above the Pt (100), (110), or (111) surfaces], for the highly symmetric sites.

visible for the hollow sites, as indicated in Figure 3. In addition, the adsorption energy of an H atom is lowest at the H, LB, and fcc-H sites, respectively, for the Pt (100), Pt (110), and Pt (111) surfaces at this height. Further, an H atom can travel along the H-B-H and H-LB-H pathways on the Pt (100) and Pt (110) surfaces, respectively, without encountering a potential barrier originating from the surface atoms at $z = 0.6$ Å and above.

We found the surface potential to be attractive for all the highly symmetrical regions at 1.2 Å height. As an H atom approaches the surface—1 Å and closer—it first encounters the potential barrier produced by the top regions, as indicated in Figures 3 and 5. The repulsive potential energy of the metal surface for an H atom increases above a top site. Figure 5 also

shows that when the H atom is at the heights 1.8 Å, 1.2 Å, and 0.6 Å above the surface, the attractive potential energy of the metal surface for the H atom increases above the bridges and hollow sites.

Figure 6 shows three-dimensional contour graphs of the potential-energy surface for side views of the Pt (100), Pt (110), and Pt (111) surfaces for an H atom in directions $y = 0$ Å and $x = 0$ Å. The effects of the potential-energy surfaces on the H atom can be seen at different heights above the surface or at different depths below the surface layers. Figures 4 and 6 show that it is feasible for an H atom to pass from the hcp-hollow site of the Pt (111) surface to the second layer and also to pass directly down to the third layer from the fcc-hollow site. The LB site is also suitable for penetration of the H atom into the

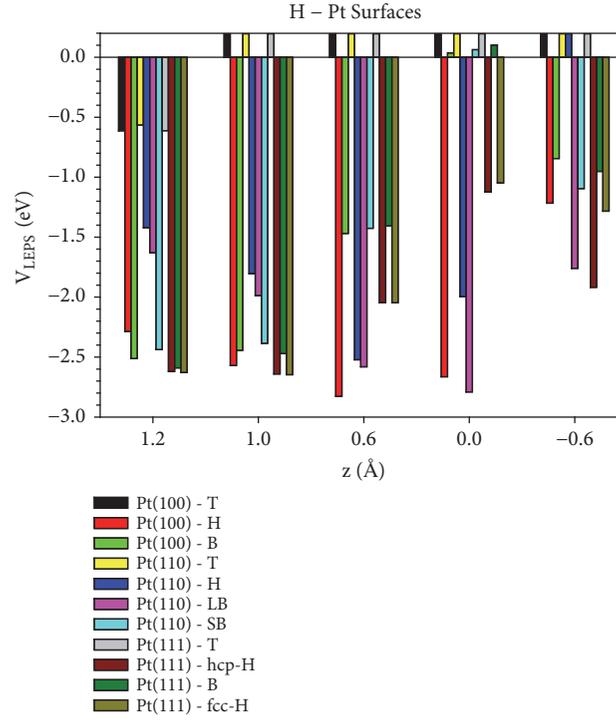


FIGURE 3: Column graph of the LEPS energy values for the highly symmetric sites on the Pt (111), (110), and (100) surfaces in the different height groups $z = -0.6, 0.0, 0.6, 1.0,$ and 1.2 \AA .

TABLE 3: Comparison of the results of this study with previous studies.

| Systems | Sites | $z \text{ (\AA)}$ | Theoretical Results $z \text{ (\AA)}$ | $E \text{ (eV)}$ | Experimental Results $E_B \text{ (eV)}$ | Theoretical Results $E_B \text{ (eV)}$ |
|-------------|-------|-------------------|--------------------------------------------|------------------|--------------------------------------------|------------------------------------------------------------------------------------------------|
| H - Pt(100) | T | 1.55 | 1.64 [14] | -2.283 | | 1.880 [14] |
| | H | 0.55 | 0.70 [14] | -2.832 | -2.565 [7] | -2.340 [14], -2.28 [28] |
| | B | 1.15 | 1.76 [12], 1.07 [14] | -2.524 | | -2.91 [12], -2.31 [14] |
| H - Pt(110) | T | 1.6 | 1.62 [14] | -2.178 | | -1.69 [14] |
| | H | 0.4 | 0.39 [14] | -2.734 | | -2.28 [14] |
| | SB | 1 | 1.03 [14] | -2.385 | | -2.22 [14] |
| | LB | 0.2 | 0.10 [14] | -2.837 | | -2.33 [14] |
| H - Pt(111) | T | 1.6 | 1.57 [13], 1.64 [14], 1.58 [25], 1.53 [26] | -2.312 | -2.78 [5] | -2.75 [13], -2.61 [13], -2.00 [14], -2.65 [25], -2.76 [26], |
| | fcc-H | 1.0 | 1.87 [12], 0.98 [25], 0.91 [26] | -2.647 | -2.456 [7], -2.643 [7], -2.63 [7] | -2.72 [12], -2.74 [13], -2.57 [13], -2.55 [14], -2.55 [19], -2.64 [22], -2.58 [25], -2.49 [26] |
| | hcp-H | 1.0 | 0.90 [26] | -2.641 | | -2.71 [13], -2.55 [13], -2.562 [14], -2.66 [26] |
| | B | 1.2 | 1.13 [25], 1.05 [26] | -2.590 | | -2.476 [14], -2.58 [25], -2.68 [26], |

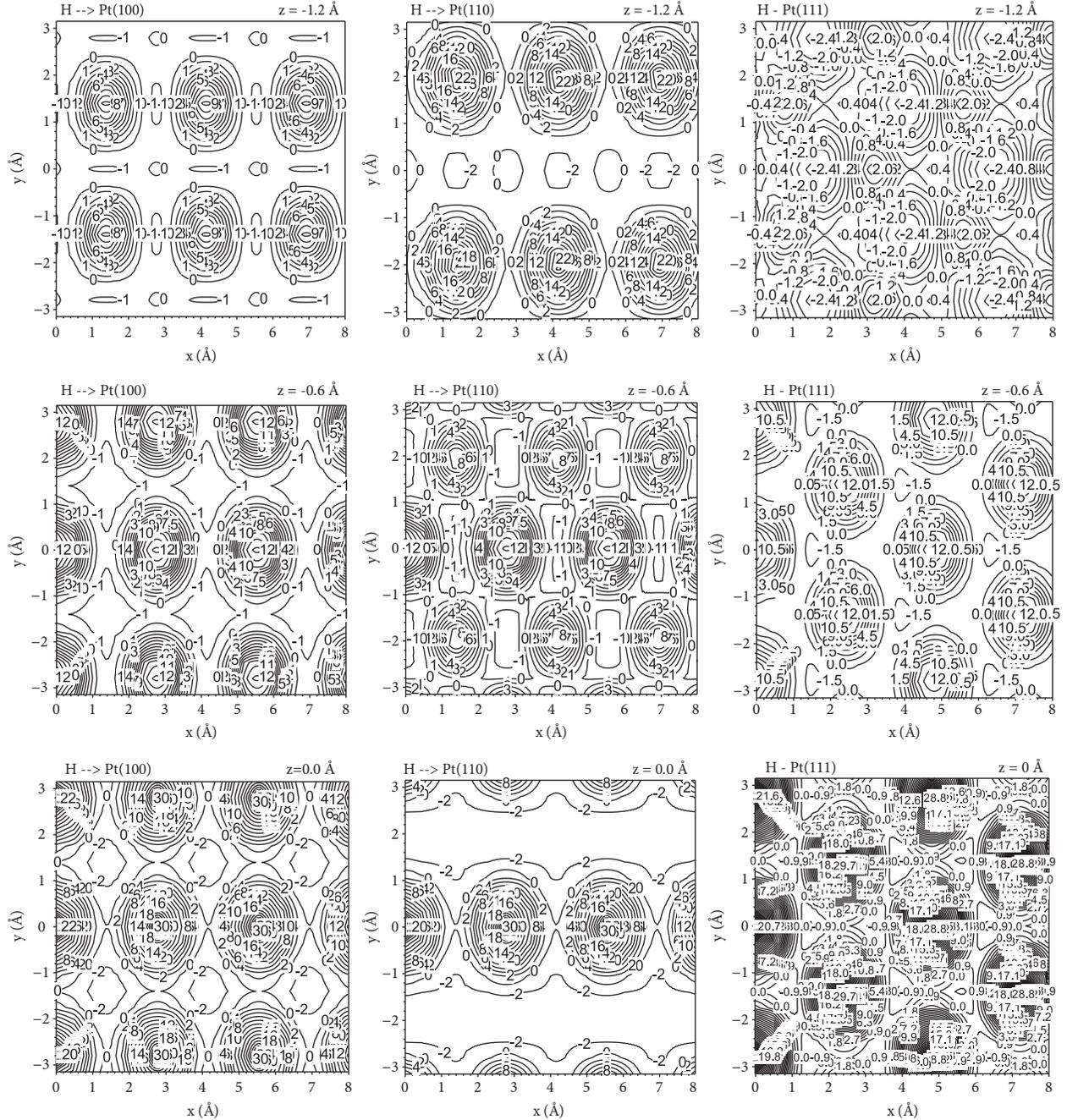


FIGURE 4: Potential-energy contours for the interaction of an H atom with Pt (111), (110), and (100) surfaces at depths $z = -1.2, -0.6$ Å, and 0.0 Å below the metal surface.

Pt (110) surface, as shown in Figure 6. Nevertheless, an H atom traveling directly to a top site over the surface encounters the high potential-energy barriers due to the surface atoms, which can scatter it back from the surface.

4. Conclusions

In the present study, we have used a LEPS potential to analyze the adsorption and diffusion of hydrogen atoms on the Pt

(100), Pt (110), and Pt (111) surfaces. The LEPS potential is particularly suitable for investigating adsorbate-surface interactions. Using this potential, we have determined theoretically the adsorption zones, penetration regions, and diffusion pathways for H atoms over each of the Pt surfaces. We found that hollow sites are more convenient for the adsorption of hydrogen atoms on the Pt (100) and Pt (111) surfaces, whereas the LB site is more suitable for the Pt (110) surface. We have also reported that the hollow sites for the three

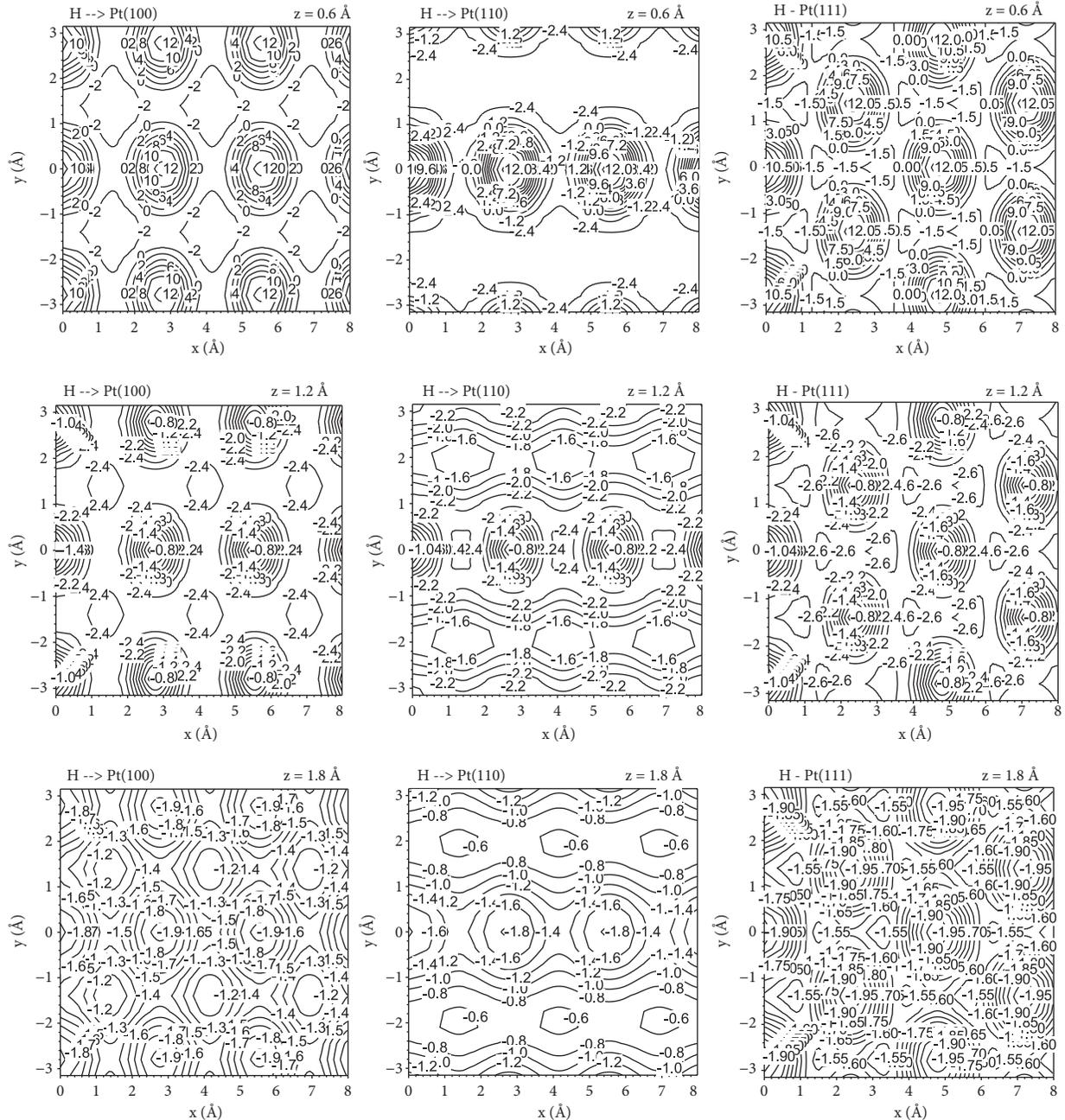


FIGURE 5: Potential-energy contours for the interaction of an H atom with the Pt (111), (110), and (100) surfaces at the heights $z = 0.6, 1.2,$ and 1.8 \AA .

surfaces are regions through which H atoms can penetrate into the subsurface, in addition to the LB site for the Pt (110) surface.

Surface diffusion is also a very important process, in which a given H atom adsorbed at a hollow site can reach a nearest-neighbor hollow site *via* a bridge site on the surface. We have found that the diffusion pathway for an H atom may follow the bridge-hollow-bridge direction on the surface at the equilibrium heights. This result shows

that while an H atom approaching a top site encounters a huge repulsive potential energy due to the surface atoms, the potential energy is attractive for the hollow sites.

Finally, we have reported that when an H atom encountering the surface has enough kinetic energy, it can penetrate into the subsurface *via* a SB site or a bridge site, in addition to passing through the hollow sites and LB sites.

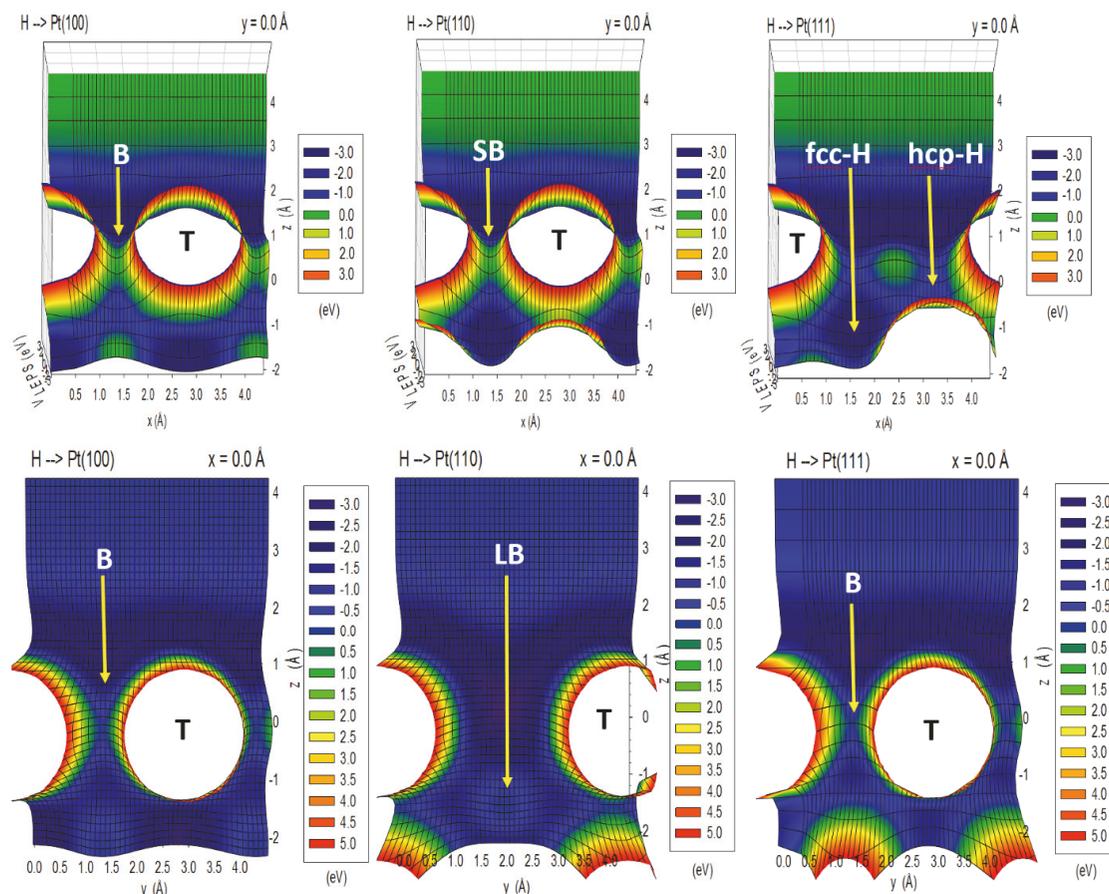


FIGURE 6: The side views of three-dimensional contour graphs of the potential-energy surface for an H atom on the Pt (111), (110), and (111) surfaces at $y = 0 \text{ \AA}$ and at $x = 0 \text{ \AA}$.

Data Availability

No external data were used to support this study. All data was calculated, tabulated, and graphed in the manuscript.

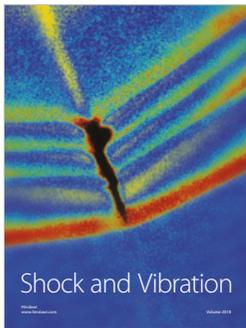
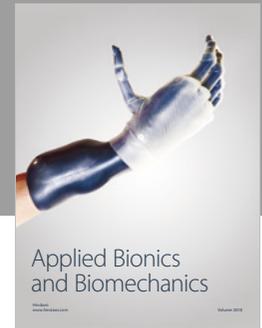
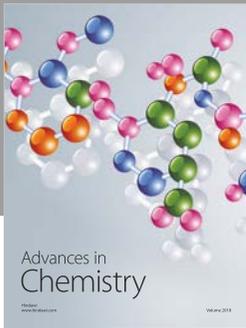
Conflicts of Interest

The author declares that there are no conflicts of interest regarding the publication of this paper.

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