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Laser Field Effect on Chemisorption Energy and Its Contributions for the System Na_2 / W(100)

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Abstract: In this study, a mathematical model is presented to study the chemisorption of two interacting atoms on solid surface in the presence of laser field. Our mathematical model is based on the occupation numbers formula that depends on the laser field which we derived according to Anderson model for single atom adsorbed on solid surface. Occupation numbers formula and chemisorption energy formula are derived for two interacting atoms (as a diatomic molecule) as they approach to the surface taking into account the correlation effects on each atom and between atoms. This model is characterized by obvious dependence of all relations on the system variables and the laser field characteristics which gives precise description for the molecule – surface interaction dynamics as a function of the normal distance from the surface and the distance between atoms .Our mathematical model is applied to the Na_2/W(100) system .It is found that the type of interaction between the atoms and surface , whether it is repulsive or attractive , is determined by the laser strength where the repulsion between the two atoms increases with the laser strength increasing. So it makes sure that the laser field can be consider as a tool to control the ionization and dissociation processes that happen on the solid surface.

Introduction

Understanding reactions on surface plays an important role in a wide range of technologically relevant applications. Among those are the heterogeneous catalysis- the majority of reactions in the chemical industry employ catalysts; crystal growth, which determines, e.g., the quality of semiconductor devices; corrosion and lubrication, which influences the durability of mechanical system; or hydrogen storage in metals, just to mention a few. The reactions involved in these processes are often too complicated to be studied in detail as a whole. Therefore in surface science one tries to understand reaction mechanisms by breaking them up into simpler steps which are then studied under well-defined conditions [1,2]. One of the early objectives of the theoretical work was to treat the simple adsorbents on the metal surface in order to understand experiments, in which adsorption was will characterized and to uncover the principle interactions that govern bonding between surface and adsorbed species [3-5]. The field of surface dynamics can be defined by the studies that directed at describing the atomic and the molecular motion and the relation between the molecular motion and the energy exchange through a surface processes such as In this study, we interest in the study of adsorption of alkali molecules on the solid surfaces because,

1- They strongly affect the surface electronic structure at sub-monolayer coverage, and reduce the surface work function [6].

2- There is an important theoretical interest in these systems because they could be considered as the simplest examples of the chemisorption.

3- Alkali molecules and metal surfaces have been investigated by the variety of experimental techniques [7].

It is hence of interest to investigate Laser-stimulated surface processes [8] which include surface excitation [9-11], desorption [12, 13], dissociation [14, 15], diffusion [16] and catalysis [17].

In this study we will study the effect the laser field on the chemisorption process of Na_2 on W(100) surface , the chemisorption energy is calculated and the effects laser field on the ionic and metallic parts are investigated considering the laser field characteristics (frequency and strength) that do not case heating or damage to the surface [18].

The Chemisorption of Diatomic Molecule in the Presence of Laser Field

In this study, a mathematical model is presented to study the chemisorption of two interacting atoms on solid surface in the presence of laser field [19] . This model is characterized by obvious dependence of all relations on the system variables and the laser field characteristics which gives precise description for the molecule – surface interaction dynamics as a function of the normal distance from the surface and the distance between atoms .Our mathematical model is applied to the Na_2 /W (100) system .It is found that the type of interaction between the atoms and surface, Figure 1.

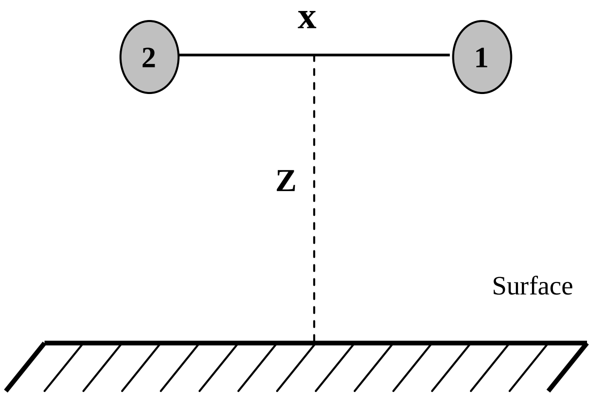

Fig. (1): Model system Na_2 / metallic surface, Z represented the normal distance between the all atom and surface and X represented the distance between two atoms.

The model Hamiltonian

We start with the following model Hamiltonian for the adsorbed-substrate system, taking the direct hopping and exchange interaction between a pair of adatoms into account [20],

$$H = H_A + H_M + H_{AM} + H_{AA} \qquad (1)$$

The first and second terms represent Hamiltonians of the adsorbate and substrate, respectively, and are giving by:

$$H_A = \sum_{\sigma}\sum_{i=1}^{2} E_i^{\sigma} n_i^{\sigma} + \sum_{i=1}^{2} U n_i^{\uparrow} n_i^{\downarrow} \qquad (2)$$

$$H_M = \sum_{\sigma}\sum_{k} E_k^{\sigma} n_k^{\sigma} \qquad (3)$$

This terms represent Hamiltonians for the unperturbed energies of the adatoms and the surface, respectively[21].

And H_{AM} and H_{AA} are those of the adsorbate-metal and adsorbate- adsorbate interaction respectively, and giving by:

$$H_{AM} = \sum_{\sigma}\sum_{k}\sum_{i=1}^{2} (V_{ik} C_{i\sigma}^{*} C_{k\sigma} + H.C) \qquad (4)$$

$$H_{AA} = \sum_{\sigma} (V_{12} C_{1\sigma}^{*} C_{2\sigma} + H.C) + \frac{1}{2} J_0 (C_{1\sigma}^{*} C_{2\sigma}^{*} C_{1\sigma} C_{2\sigma} + H.C) \qquad (5)$$

V_{ik} and V_{12} the hopping integrals ϕ_k^{σ} and ϕ_i^{σ} are the orbital energies of E_k^{σ} And E_i^{σ} between ϕ_i^{σ} and ϕ_k^{σ} and between ϕ_2^{σ} and ϕ_1^{σ} respectively .

U is the intratomic Coulombic interaction energy in an adatom, and J_o the exchange integral between adatoms [20]. One can give a good description to the molecular adsorption by introducing the effective exchange term. This term is defined as the combination of the three integral [21],

$$J = J_0 + 2SV_{12} \qquad (6)$$

Two specific cases may be discussed depending on the values of J, these are:

1- For large negative values of J, the binding energy between the two adatoms become repulsive near the surface and the molecule may dissociate at the surface.

2- For intermediate negative or for positive values of J the net interaction will be attractive [21]. The indirect interaction V_{ik} may be written as $\lambda_{12}^{\pm\sigma}$ which defined by Alexander and Anderson [22], could be modified to include the molecule separation from the surface as,

$$\lambda_{12}^{\pm\sigma}(E, Z, X) = -i\Delta_i^{\sigma}(E, Z)\sin(KX)/KX \qquad (7)$$

Where, K is defined by E_k^σ, since E_k^σ is the energy of an electron with momentum k and spin, k is taken to be equal to $\sqrt{2u_o}$, with u_o represents the bottom conduction band. And σ is the levels half width around each atom .The energy dependence of the half width $\Delta_i^\sigma(z)$ was neglected while the spin and the distance dependence [21], and the explicit dependence on the molecule-metal separation can be approximated to the fallowing analytical formula [23-25],

$$\Delta_i^\sigma(z) = \frac{(q_i^{\pm\sigma})^2}{16V_0(z+r_i)}\sqrt{2V_0-(q_i^{\pm\sigma})^2}\left[1+\frac{1}{2(z+r_i)q_i^{\pm\sigma}}\right]e^{-2zq_i^{\pm\sigma}} \tag{8}$$

with $q_i^{\pm\sigma} = \sqrt{2\left|E_i^{\pm\sigma}\right|}$ since $V_O = \phi + |u_o|$ i=1,2 , and r_i is the standard radius for the alkali ions .

Depending on the relation (1) the atomic levels of the two atoms (1, 2) are written as [20]:

$$E_1^{\pm\sigma} = E_i^\infty + Un_1^{\mp\sigma} - Jn_2^{\pm\sigma} \tag{9}$$

$$E_2^{\pm\sigma} = E_2^\infty + Un_2^{\mp\sigma} - Jn_1^{\pm\sigma} \tag{10}$$

$n_1^{\pm}, n_2^{\pm\sigma}$ represent the average occupation numbers of the E_i^∞ states around the adatoms. $E_i^{\pm\sigma}$ is given by the following equation:

$$E_1^\infty = E_2^\infty = \Phi - V_I \tag{11}$$

represent the surface work function and ionization level of the adatom, respectively.

The occupation numbers

The occupation number of the adatom (1, 2) is written as [24]:

$$n_i^\sigma = \int_{u_0}^{E_F} \rho_i^\sigma(E)dE \tag{12}$$

$E_F, \rho_i^{\pm\sigma}$ represent the Fermi level and the local density of states on the adatoms i, of spin σ [19].

$$\rho_1^{\pm\sigma}(E) = \frac{1}{2\pi}\left(\frac{(1+Y^{\pm\sigma}/V^{\pm\sigma})\Delta_1^{\pm\sigma}}{(E-E_+^{\pm\sigma})^2+(\Delta_1^{\pm\sigma})^2} + \frac{(1-Y^{\pm\sigma}/V^{\pm\sigma})\Delta_1^{\pm\sigma}}{(E-E_-^{\pm\sigma})^2+(\Delta_1^{\pm\sigma})^2}\right) \tag{13}$$

$$\rho_2^{\pm\sigma}(E) = \frac{1}{2\pi}\left\{\frac{(1-Y^{\pm\sigma}/V^{\pm\sigma})\Delta_2^{\pm\sigma}}{(E-E_+^{\pm\sigma})^2+(\Delta_2^{\pm\sigma})^2} + \frac{(1+Y^{\pm\sigma}/V^{\pm\sigma})\Delta_2^{\pm\sigma}}{(E-E_-^{\pm\sigma})^2+(\Delta_2^{\pm\sigma})^2}\right\} \tag{14}$$

Where the operative definition of $E_\pm^{\pm\sigma}$ can be expressed as,

$$E_+^{\pm\sigma} = E_i + \Delta E_{img} + Un^{\mp\sigma} - Jn^{\pm\sigma} + V^{\pm\sigma} \tag{15}$$

$$E_-^{\pm\sigma} = E_i + \Delta E_{img} + Un^{\mp\sigma} - Jn^{\pm\sigma} - V^{\pm\sigma} \tag{16}$$

E_{img} Represent the image shift. It is added to the atomic energy level as an energy shift of atom (i) The variation of this shift with normal distance from the surface is given by [26],

$$\Delta E_{img} = \frac{e^2}{4(z+z_o)} \tag{17}$$

Z_o is the screening length, and it is taken to be (2.4 + r_i) A°. The variation of screening with laser field parameters is not taken into account in our treatment.

And

$$V^{\pm\sigma} = \sqrt{V_{12}^2+(Y^{\pm\sigma})^2} \tag{18}$$

$$V_{12}^{\sigma^2} = \left|V_{12}+\lambda_{12}^{\pm\sigma}\right|^2 \tag{19}$$

$$Y^{\pm\sigma} = Ud^{\mp\sigma} + Jd^{\pm\sigma} \tag{20}$$

And, d^σ and n^σ are defined as,

$$d^\sigma = \frac{1}{2}(n_1^\sigma - n_2^\sigma) \tag{21}$$

$$n^\sigma = \frac{1}{2}(n_1^\sigma + n_2^\sigma) \tag{22}$$

By used the formalism of the density of states around one atom [27] and the formalism of density of states in the relation (13), we can be write[19]:

$$\rho_1^\sigma(E) = \sum_{n=0,\pm1}\sum_{j=+,-} C_{nj1}^\sigma \frac{\Delta_{T_1}^\sigma}{(E-E_j^\sigma+n\hbar\omega)^2+(\Delta_{T_1}^\sigma)^2} \tag{23}$$

Where J= +, - , refer of the energy E_j^σ which are defined in relations (15), (16) by $E_+^{\pm\sigma}$ and , and the functions C_{nj1}^σ are,

$$C_{0j1}^\sigma = \frac{1}{2\pi}(1+j\frac{Y^\sigma}{V^\sigma})\frac{\Delta_1^\sigma}{\Delta_{T_1}^\sigma} \tag{24}$$

$$C_{-1j1}^\sigma = \frac{1}{2\pi}(1+j\frac{Y^\sigma}{V^\sigma})\frac{\Delta_L}{\Delta_{T_1}^\sigma} \tag{25}$$

$$C_{+1j1}^\sigma = C_{-1j1}^\sigma \tag{26}$$

And substituting eq.(23) into eq.(12) and solving these equations analytically , we get

$$n_1^{\sigma} = \sum_{n=0,\pm1}\sum_{j=-,+} C_{nj1}^{\sigma}\left\{\tan^{-1}\frac{(E_F - E_j^{\sigma} + n\hbar\omega)}{\Delta_{T_1}^{\sigma}} - \tan^{-1}\frac{(u_0 - E_j^{\sigma} + n\hbar\omega)}{\Delta_{T_1}^{\sigma}}\right\} \qquad (27)$$

Where, $\Delta_{T_1}^{\sigma}$ is defined by [27].

(i=1,2) $\Delta_{T_1}^{\sigma} = \Delta_i^{\sigma} + 2\Delta_L$

$\Delta_i^{\pm\sigma}$ as defined in eq.(8) is the important parameter in determining the chemisorption energy.

And Δ_L represent the broadening by laser field effect, it is given by the following form as function of Z

$$\Delta_L = \Delta_{0L} e^{-4\alpha_L Z} \qquad (28)$$

With $\alpha_L = \sqrt{2|V_I|}$ (in a.u.) [24] and Δ_{0L} represent the broadening at Z = 0A^0 , i.e. on the surface where they take their maximum values . where Δ_{0L} is equal to $\Pi\bar{\rho}W_L^2$. and W_L represent the strength of laser field .

In the same way, we found the formalism of the occupation numbers around the adatom (2) . We get ,

$$\rho_2^{\sigma}(E) = \sum_{n=0,\pm1}\sum_{\left(\substack{j=+,m=-\\ j=-,m=+}\right)} C_{nj2}^{\sigma}\frac{\Delta_{T_2}^{\sigma}}{\left(E - E_m^{\sigma} + n\hbar\omega\right)^2 + \left(\Delta_{T_2}^{\sigma}\right)^2} \qquad (29)$$

So that,

$$n_2^{\sigma} = \sum_{n=0,\pm1}\sum_{\left(\substack{j=+,m=-\\ j=-,m=+}\right)} C_{nj2}^{\sigma}\left\{\tan^{-1}\frac{(E_F - E_m^{\sigma} + n\hbar\omega)}{\Delta_{T_2}^{\sigma}} - \tan^{-1}\frac{(u_0 - E_m^{\sigma} + n\hbar\omega)}{\Delta_{T_2}^{\sigma}}\right\} \qquad (30)$$

Chemisorption energy of the two interacted adatoms

The chemisorption energy, $E_{ch}(V_{12},J)$, in general, is defined as being the difference between the final and the initial energies of the system . According to Anderson model, the chemisorption energy is the change in the ground state energy on switching on the coupling assuming one electron on the adatoms initially. In general, the chemisorption energy is divided into two parts. These are the metallic part and the ionic part [28].

The metallic part of the bond energy, which may be called delocalization energy, results from allowing the valance electron of the adatom to spread throughout the metal and the metal electrons to spread a bit into the region of the adatom. This part of chemisorption energy is given by [29].

$$E_M(V_{12},J) = \sum_{\sigma}\sum_{i}\int_{u_0}^{E_F} E\rho_i^{\sigma}(E)dE - \sum_{i=1}^{2} U n_i^{\sigma} n_i^{-\sigma} + J\sum_{\sigma} n_1^{\sigma} n_2^{\sigma} \qquad (31)$$

Then, by substituting the formula of local density of states on the adatoms in the presence of laser field eq.(13), eq(14) into eq.(31) , we get [19]

$$E_M(V_{12},J) = \sum_{\sigma}\left[\sum_{n=0,\pm1}\sum_{j=+,-} C_{nj1}^{\sigma}\Delta_{T_1}^{\sigma}\int_{u_0}^{E_F}\frac{E}{\left(E - E_j^{\sigma} + n\hbar\omega\right)^2 + \left(\Delta_{T_1}^{\sigma}\right)^2}dE + \sum_{n=0,\pm1}\sum_{\left(\substack{j=-,m=+\\ j=+,m=-}\right)} C_{nj2}^{\sigma}\Delta_{T_2}^{\sigma}\int_{u_0}^{E_F}\frac{E}{\left(E - E_m^{\sigma} + n\hbar\omega\right)^2 + \left(\Delta_{T_2}^{\sigma}\right)^2}dE\right] - \sum_{i=1}^{2} U n_i^{\sigma} n_i^{-\sigma} + J\sum_{\sigma} n_1^{\sigma} n_2^{\sigma} \qquad (32)$$

And by doing the integration on energy that encloses the occupied states below the Fermi level E_F, one gets [19].

$$\begin{aligned}
E_M(V_{12},J) = {} & \sum_{\sigma}\sum_{n=0,\pm1}\sum_{j=+,-} C_{nj1}^{\sigma}\left(E_j^{\sigma} - n\hbar\omega\right)\left\{\tan^{-1}\frac{E_F - E_j^{\sigma} + n\hbar\omega}{\Delta_{T_1}^{\sigma}} - \tan^{-1}\frac{u_0 - E_j^{\sigma} + n\hbar\omega}{\Delta_{T_1}^{\sigma}}\right\} \\
& + \sum_{\sigma}\sum_{n=0,\pm1}\sum_{j=+,-} C_{nj1}^{\sigma}\frac{\Delta_{T_1}^{\sigma}}{2}\ln\left[\frac{\left(E_F - E_j^{\sigma} + n\hbar\omega\right)^2 + \left(\Delta_{T_1}^{\sigma}\right)^2}{\left(u_0 - E_j^{\sigma} + n\hbar\omega\right)^2 + \left(\Delta_{T_1}^{\sigma}\right)^2}\right] \\
& + \sum_{\sigma}\sum_{n=0,\pm1}\sum_{\left(\substack{j=+,m=-\\ j=-,m=+}\right)} C_{nj2}^{\sigma}\left(E_m^{\sigma} - n\hbar\omega\right)\left\{\tan^{-1}\frac{E_F - E_m^{\sigma} + n\hbar\omega}{\Delta_{T_2}^{\sigma}} - \tan^{-1}\frac{u_0 - E_m^{\sigma} + n\hbar\omega}{\Delta_{T_2}^{\sigma}}\right\}
\end{aligned}$$

$$+\sum_{\sigma}\sum_{n=0,\pm1}\sum_{\begin{pmatrix} j=+,m=- \\ j=-,m=+ \end{pmatrix}} C^{\sigma}_{nj2}\frac{\Delta^{\sigma}_{T_2}}{2}\ln\left[\frac{\left(E_F-E^{\sigma}_{m}+n\hbar\omega\right)^2+\left(\Delta^{\sigma}_{T_2}\right)^2}{\left(u_0-E^{\sigma}_{m}+n\hbar\omega\right)^2+\left(\Delta^{\sigma}_{T_2}\right)^2}\right]$$

$$-U\sum_{i} n_i^{\sigma} n_i^{-\sigma} + J\sum_{\sigma} n_1^{\sigma} n_2^{\sigma} \qquad (33)$$

In the right side in eq.(33) , the first and second terms are for adatom 1 , and the third and the fourth terms are for atom 2. The fifth and sixth terms the chemisorption energy due to intra-atomic interaction in each adatom and the effective exchange interaction (interatomic interaction) between the two adatoms respectively.

Note that in eq.(33), the laser field effect is added explicitly to the molecule energy levels positions and the broadening function .

The ionic energy is the energy associated with bringing a charge infinitely removed from the metal up to a distance Z from the surface and it is given by [30].

$$W(Z) = -e^2\int_{\infty}^{z}\frac{z^2_{eff}(z')dz}{4(z'+z_0)^2} \qquad (34)$$

Where, the z_{eff} (z') is the Z-dependent effective charge on the molecule, and it may be

$$z_{eff}(z) = 2-\sum_{i}(n_i^{\sigma}(z)+n_i^{-\sigma}(z))$$

Finally, eqs.(33) and (34) are calculated numerically to get the total chemisorption energy,

$$E_{che}(V_{12},J) = E_M + W(z) \qquad (35)$$

The main purpose of this application is to calculate the chemisorption energy E_{che} (ionic part and metallic part), between a pair of Na-atom (V_I=5.14eV and V_A=0.74eV) as they approach to the W(100) $\hbar\omega = 1,3,5eV$ surface [31] and adsorbed on it with strength of laser field W_L= 2.7, 5.4 eV. and frequency $\phi = 4.58eV$ The system of the coupled equations

$$n_1^{\pm\sigma}, n_2^{\pm\sigma}, E_1^{\pm\sigma}, E_2^{\pm\sigma}$$

Solved-consistently. All the chemisorption functions are calculated and investigated as a function of both atom- atom intermolecular distance and the molecular normal distance above the surface.

The initial conditions at large distance (Z=10 A^{o}) from the surface are:

$$\begin{aligned} n_1^{\sigma} &= n_2^{\sigma} = 1 \\ n_1^{-\sigma} &= n_2^{-\sigma} = 0 \end{aligned} \qquad (36)$$

And the atomic levels at the same distance are calculated from,

$$\begin{aligned} E_1^{\sigma} &= E_2^{\sigma} = (\phi - V_I) - J \\ E_1^{-\sigma} &= E_2^{-\sigma} = (\phi - V_I) + U \qquad 2 \le X \le 6.2A^0 \end{aligned}$$

Results and Conclusion

Our model calculation gives the occupation numbers and all the related chemisorption function [19] as well as the chemisorption energy and its ionic and metallic parts for the system Na_2 / W (100) as a function of 2≤X≤6.2A^{o} at Z=0A^{0} and laser field parameters . All these result give as precise description for the ionization of the interacting adatoms

Table (1) presents the occupation number at Z=0 A^{0} as a function of the distance between the adatoms as well as the laser field parameters W_L and $\omega\hbar$. At the surface, the adatoms are in nonmagnetic state where $n_i^{\sigma}=n_i^{-\sigma}$ and $n_1^{\pm\sigma}=n_2^{\pm\sigma}$ The occupation numbers are decreasing as X is increasing for certain W_L and $\omega\hbar$. Also for certain X and field strength they decrease as increase. The increasing of field strength increases the ionization of the interacting adatoms.

Table (2),(3) and (4) represent the ionic , metallic and the chemisorption energies respectively as a function of all the parameters that are our mentioned of table (1). For certain W_L and $\omega\hbar$, the ionic energy increases with X , but for certain W_L , this energy increases with for X=2 A^{0} and decreases for X=6.2 A^{0} .While for the metallic part, for certain W_L and $\omega\hbar$, this energy decreases with X , but for certain W_L it increases with $\omega\hbar$ for X= 6.2 A^{0} and decreases for X=2 A^{0} .In general the metallic part is dominant in the presence and absence of laser field. So the behavior of the chemisorption energy follows the metallic part one.

Finally, one can conclude that the laser field can be used as a tool to increase the ionization of the interacting alkali adatoms and to reduce the ionic and metallic parts of the chemisoption energy, i.e the laser field reduces the chemisorption energy. This enhances the bonding breaking between the adatoms and between each atom and the surface which lead to the dissociation process.

Table (1): Shows the occupation number as a function of $W_L, \hbar\omega, X$ at Z=0Ao

$X(A^o)$	$n_1^{+\sigma} = n_1^{-\sigma} = n_2^{+\sigma} = n_2^{-\sigma}$ at $(Z=0)$						
	In the absence of laser field	$W_L = 2.7eV$			$W_L = 5.4\,eV$		
		$\hbar\omega = 1eV$	$\hbar\omega = 3eV$	$\hbar\omega = 5eV$	$\hbar\omega = 1eV$	$\hbar\omega = 3eV$	$\hbar\omega = 5eV$
2.0992	0.49995	0.40649	0.39551	0.36733	0.24659	0.24316	0.23666
4.0988	0.49950	0.34059	0.32929	0.33966	0.25144	0.24968	0.24654
6.200	0.49637	0.27027	0.30996	0.35531	0.24806	0.24766	0.24623

Table (2): Shows the ionic part energy as a function of $W_L, \hbar\omega, X$ at Z=0Ao

$X(A^o)$	$W(Z=0)$ (ev)						
	In the absence of laser field	$W_L = 2.7\,eV$			$W_L = 5.4\,eV$		
		$\hbar\omega = 1eV$	$\hbar\omega = 3\,eV$	$\hbar\omega = 5\,eV$	$\hbar\omega = 1eV$	$\hbar\omega = 3\,eV$	$\hbar\omega = 5\,eV$
2.0992	-3.42E-9	-0.00911	-0.01197	-0.0236	-0.09049	-0.09963	-0.12488
4.0988	-3.27E-7	-0.05656	-0.56974	-0.24163	-0.14107	-0.59409	-0.29395
6.200	-0.9414	-1.07388	-0.73348	-0.21292	-0.96870	-0.70478	-0.2401

Table (3): Shows the metallic part energy as a function of $W_L, \hbar\omega, X$ at Z=0Ao

$X(A^o)$	$E_M(Z=0)$ (eV)						
	In the absence of laser field	$W_L = 2.7eV$			$W_L = 5.4eV$		
		$\hbar\omega = 1eV$	$\hbar\omega = 3eV$	$\hbar\omega = 5eV$	$\hbar\omega = 1eV$	$\hbar\omega = 3eV$	$\hbar\omega = 5eV$
2.0992	-15.9217	-12.462	-12.1872	-11.1183	-7.56042	-7.71595	-7.7303
4.0988	-3.67927	-6.82583	-7.65776	-8.9665	-7.48996	-7.69301	-7.87536
6.200	-0.11637	-5.18516	-6.16718	-7.88877	-7.30362	-7.45181	-7.63116

Table (4): Shows the Chemisorption energy as a function of $W_L, \hbar\omega, X$ at Z=0Ao

$X(A^o)$	$E_{che}(Z=0)$ (eV)						
	In the absence of laser field	$W_L = 2.7eV$			$W_L = 5.4eV$		
		$\hbar\omega = 1eV$	$\hbar\omega = 3eV$	$\hbar\omega = 5eV$	$\hbar\omega = 1eV$	$\hbar\omega = 3eV$	$\hbar\omega = 5eV$
2.0992	-15.9217	-12.4711	-12.1992	-11.14119	-7.65091	-7.81558	-7.85518
4.0988	-7.67927	-6.88239	-8.2275	-9.20813	-7.63103	-8.28707	-8.16931
6.200	-1.05781	-6.25909	-6.90066	-8.10169	-8.27241	-8.15659	-7.87126

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تأثير مجال الليزر على طاقة الالتصاق الكيميائي ومساهماتها لنظام Na_2 / W(100)

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الخلاصة: قدم في هذه الدراسة أنموذج حسابي لدراسة الالتصاق الكيميائي لذرتين متفاعلتين على سطح الصلب بوجود مجال الليزر . أعتمد أنموذجنا الحسابي على صيغة أعداد الإشعال(المشغولة) المعتمدة على مجال الليزر والتي اشتقت وفق أنموذج أندرسن لذرة منفردة على الالتصاق بالسطح الصلب . حيث اشتقت صيغة لأعداد الإشغال وكذلك طاقة الالتصاق الكيميائي للذرتين المتفاعلتين باعتبار(الجزيئة ثنائية الذرة) قريبتين من السطح أخذين بنظر الاعتبار تأثيرات التبادل على كل ذرة بين الذرتين . تميز هذا النموذج بوضوح اعتماد العلاقات على كل المتغيرات التي تخص النظام ومواصفات مجال الليزر والذي يعطي وصفاً دقيقاً لديناميكية تفاعل جزيئه – سطح كدالة للمسافة العمودية بين الجزيئه والسطح والمسافة بين الذرتين المتفاعلتين . طبق أنموذجنا الحسابي لنظام Na_2 / W(100)، و وجد أن لشدة مجال الليزر تأثيراً على حالة التفاعل بين الذرتين والسطح فيما إذا كان التفاعل تنافري او تجاذبي . إذا يزداد التنافر بين الذرتين كلما ازدادت شدة مجال الليزر. وعلية يصبح من المؤكد أن مجال الليزر يعتبر أداة للتحكم في عمليتي التأين والتفكك التي تحدث على السطح الصلب.