CHARACTERIZATION OF NANOCRYSTALLINE SILICON GERMANIUM FILM AND NANOTUBE IN ADSORPTION GAS BY MONTE CARLO AND LANGEVIN DYNAMIC SIMULATION

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ABSTRACT. The nanocrystalline silicon-germanium films (Si/Ge) and Si/Ge nanotubes have low band gaps and high carrier mobility, thus offering appealing potential for absorbing gas molecules. Interaction between hydrogen molecules and bare as well as functionalized Si/Ge nanofilm and nanotube was investigated using Monte Carlo (MC) and Langevin dynamic (LD) simulation methods. It was found that the binding energy of the H_2 on the Si/Ge surface is weak, and be enhanced by increasing curvature of surface to tube form and increasing temperature. The structural, total energy and energy band gaps of H_2 absorbed nanocrystalline silicon germanium film (Si/Ge) and as it passes through Si/Ge nanotube was also studied. They are computed with MC and LD simulation the methods at different temperatures. All the calculations were carried out using HyperChem 7.0 program package.

KEY WORDS: Monte Carlo, Langevin dynamic simulation, Silicon-germanium films (Si/Ge), Si/Ge nanotube

INTRODUCTION

Si/Ge nanostructures are considered as candidates with high potential for integration into many nanoengineered systems. Moreover, their integration into micro-electric mechanical system (MEMS) opens new routes for the fabrication of ever faster and sensitive devices. Thus one key element is the development of methods to fabricate three-dimensional Ge/Si micro- and nano-objects (MNOs) and controls their size accurately [1]. Careful comparison of silicon and germanium chemical properties, however, shows subtle but indisputable differences, with Ge exhibiting distinct lithopile, siderophile or organophile behavior depending on its environment [2]. These specific properties are responsible for Ge geochemical cycles in the ocean and continental environments not being simple analogues of corresponding silica cycles [3]. This requires Ge to be enriched in the secondary phases that form during the weathering of primary silicates.

Si/Ge is used for the adsorption of gases that is to form nanofilm and nanotube (Figure 1). It is important to study the e-beam induced phenomena in silica based glasses because germanium doped silica is one of the most used optical materials for production of integrated optical devices in which e-beam writing is foreseen. The integrated circuit fabrication by direct e-beam writing offers several advantages compared to the traditional photolithography techniques, in particular its large flexibility which allow the mastering of section of refractive index waveguides [4].
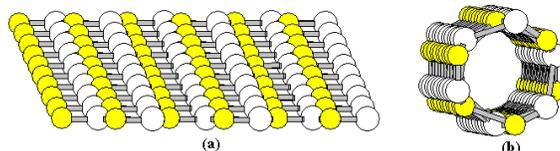

Figure 1. Optimized configuration top-view (⬤Si/◯Ge) nanofilm and (⬤Si/◯Ge) nanotube.

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Following the observation of strong visible luminescence at room temperature from porous Si (PS) [5], several groups also attempted to prepare porous Si/Ge (PSG) with visible luminescence, either by anodization or stain etching [6]. The second observation makes PSG a more attractive material than PS for both fundamental research and industrial applications.

However, further detailed investigations are required to determine the properties of such films and tubes that evaluate their potential for future application in technologies compatible with main stream Si/Ge technology [1]. The sealed silica tube method is known as the most convenient and simplest ways for the preparation of sulfide compounds from the mixture of an element and sulfur. There is a lot of information available about the syntheses of sulfides by that method in the literature [7].

A classical example of a heterogeneous chemical reaction is recombinative desorption of two atoms from well-defined surfaces. In the elementary case the process involves a breaking of two adatom-surface bonds and formation of a diatomic molecule with a single new atom–atom bond [8]. However, such a trivial description of the process can neglect the role of a solid surface. Effects such as reconstruction of a surface, the local modification of electronic states or even the formation or breaking of chemical bonds between surface atoms can essentially influence energetic and dynamics of reactions and complicate the above mentioned elementary model. (While for metals the consideration of such effects is complicated, weakening or even breaking of bonds on a covalent solid surface is identified much easier.) In this connection a ''hydrogen – Si/Ge'' system is an excellent example [9].

Hydrogen is an elementary adsorbate and at the same time it plays an important technological role. However, despite of intensive experimental and theoretical study of hydrogen interaction with a silicon surface, the details of mechanisms of H_2 adsorption and desorption from a Si/Ge surface remain contradictory. The basic contradiction is the first order of desorption kinetics and its recombinative character (hydrogen desorbs only in molecular form H_2) [10] has required a detailed discussion of the desorption mechanism. From the recently proposed models it is necessary to note, for example, a desorption mediated by surface defects [11], concerted desorption from ''pre-paired'' configuration, the mechanism of irreversible excitation of hydrogen molecules in the delocalized state. Another contradiction is a very low sticking coefficient of molecular hydrogen, which assumes a high adsorption barrier, while in desorption experiments and theoretical calculations such which assumes a high adsorption barrier, while in desorption experiments and theoretical calculations such barrier was not observed. The influence of surface coverage on the character of interaction with hydrogen is not widely studied yet [12].

EXPERIMENTAL

Computational details

There are three steps in carrying out any quantum mechanical calculation in HyperChem 7.0 program package [13]. First, prepare a molecule with an appropriate starting geometry. Second, choose a calculation method and its associated (Setup menu) options. Third, choose the type of calculation (single point, geometry optimization, molecular dynamics, Langevin dynamics, Monte Carlo, or vibrational analysis) with the relevant (Compute menu) options. These geometry optimization calculations can use either molecular mechanics or quantum mechanics to further refine the molecular geometry beyond that given by the Model Builder.

HyperChem uses the Metropolis method [14], which chooses random configurations with this probability, to concentrate sampling of configurations in regions of space that make important contributions to the calculation of thermodynamic averages.

Langevin dynamics (LD) simulation

The Langevin equation is a stochastic differential equation in which two force terms have been added to Newton's second law to approximate the effects of neglected degrees of freedom [15]. These simulations can be much faster than molecular dynamics. The molecular dynamics method is useful for calculating the time dependent properties of an isolated molecule. However, more often, one is interested in the properties of a molecule that is interacting with other molecules. With HyperChem, we can add solvent molecules to the simulation explicitly, but the addition of many solvent molecules will make the simulation much slower. A faster solution is to simulate the motion of the molecule of interest using Langevin dynamics. Langevin dynamics simulates the effect of molecular collisions and the resulting dissipation of energy that occur in real solvents, without explicitly including solvent molecules. This is accomplished by adding a random force (to model the effect of collisions) and a frictional force (to model dissipative losses) to each atom at each time step. Mathematically, this is expressed by the Langevin equation of motion:

$$\frac{\vec{F_i}}{m_i} - \gamma_i \vec{v_i} + \frac{\vec{R_i}(t)}{m_i} = \vec{a_i} \tag{1}$$

Here, $\vec{F_i}$ is force on each atom as a function of time, γ_i is the friction coefficient of the solvent, in units of ps^{-1}, and $\vec{R_i}$ is the random force imparted to the solute atoms by the solvent and the change in velocities, $\vec{v_i}$, is equal to the integral of acceleration over time. The friction coefficient is related to the diffusion constant D of the solvent by Einstein's relation:

$$\gamma_i = \frac{K_B T}{mD}.$$

The random force is calculated as a random number, taken from a Gaussian distribution, with an average value of zero and no correlation with the atom's velocity.

Integration algorithm

To integrate the Langevin equation, HyperChem uses the method [16] of:

$$r(t+\Delta t) = r(t) + c_1 \Delta t v(t) + c_2 \Delta t^2 F(t)/m + \Delta r^G \tag{2}$$

$$v(t+\Delta t) = c_0 v(t) + c_1 \Delta t F(t)/m + \Delta v^G \tag{3}$$

where, if the atomic positions at a particular time, *t*, are $r(t)$, the velocities, $v(t)$ are the first derivative of the positions with respect to time

$c_0 = e^{-t}$

$c_1 = (1 - c_0)/(\gamma \Delta t)$

$c_2 = (1 - c_1)/(\gamma \Delta t)$

That Δr^G and Δv^G are random numbers chosen from a Gaussian distribution, with:

$\langle \Delta r^G \rangle = 0$

$\langle \Delta v^G \rangle = 0$

And standard deviations:

$$\sigma_r^2 = \Delta t^2 (k_B T/m)(\gamma \Delta t)^{-1}(2 - (\gamma \Delta t)^{-1}(3 - 4 e^{-\gamma \Delta t} + e^{-2\gamma \Delta t})) \tag{4}$$

$$\sigma_v^2 = (k_B T/m)(1 - e^{-2\gamma\Delta t})$$
(5)

σ_r and σ_v are correlated, with correlation coefficient c_{rv}, defined through the relation:

$$c_{rv}\sigma_r\sigma_v = \Delta t (k_B T/m)(\gamma\,\Delta t)^{-1}(1 - e^{-2\gamma\Delta t})$$
(6)

Assuming that the interatomic force term F(t) varies linearly with time, the equations above can be rewritten in a form which produces more accurate simulations:

$$r(t + \Delta t) = r(t) + c_1\Delta t v(t) + c_2\Delta t^2 F(t)/m + \Delta r^G$$
(7)

$$v(t + \Delta t) = c_0 v(t) + (c_1 - c_2)\Delta t F(t)/m + c_2\Delta t F(t + \Delta t)/m + \Delta v^G$$
(8)

as γ approaches zero, this method reduces to the velocity Verlet algorithm:

$$r(t+\Delta t) = r(t) + \Delta t v(t) + \tfrac{1}{2}\Delta t^2 F(t)/m$$
(9)

$$v(t+\Delta t) = v(t) + \tfrac{1}{2}\Delta t[F(t)+F(t+\Delta t)/m]$$
(10)

In general, Langevin dynamics simulations run much the same as molecular dynamics simulations. There are differences due to the presence of additional forces. Most of the earlier discussions on simulation parameters and strategies for molecular dynamics also apply to Langevin dynamics, exceptions and additional considerations are noted below.

Molecular mechanics (Monte Carlo simulation)

The Metropolis implementation of the Monte Carlo algorithm has been developed by studying the equilibrium thermodynamics of many-body systems. Choosing small trial moves, the trajectories obtained applying this algorithm agree with those obtained by Langevin's dynamics [17]. With effectively search in the resultant energy landscape, we exploited the recently developed parallel hyperbolic sampling algorithm in our Monte Carlo (MC) simulations. Previously, this protocol was shown to be more effective than general replica sampling in searching for low-energy structures. Especially the energy landscape is significantly more rugged for proteins of large size than the energy landscape of small proteins [18]. This is understandable because the Monte Carlo simulations always detect the so-called "important phase space" regions which are of low energy [19]. Because of imperfections of the force field, this lowest energy basin usually does not correspond to the native state in most cases, so the rank of native structure in those decoys produced by the force field itself is poor. Therefore, the rank of native structure could be relatively better when ranked by the second force field [20]. In order to compute the average properties from a microscopic description of a real system, one should evaluate integrals over phase space. It may be calculated for an *N*-particle system in an ensemble with distribution function $P(r^N)$, the experimental value of a property $A(r^N)$ from:

$$\langle A(r^N)\rangle = \int A(r^N)P(r^N)dr^N$$
(11)

The problem with direct evaluation of this multi-dimensional integral (apart of the huge number of phase space points as a sample) is that most of the configurations sampled contribute nothing to the integral. Having energy is so high that the probability of their occurrence is vanishingly small. The trick, then, is to generate trajectories sample commonly occurring configurations more than rare ones.

For LD and MC calculation the energies are essentially the only quantities available from a single point calculation. An analysis of the components of this molecular mechanics energy is placed in the log file for further detail. In the case of MM$^+$, a much more complete description of the individual contributions to the energy, including individual stretch energies, bending energies, etc., is placed in the log file along with the system dipole moment, if bond dipoles are available.

RESULTS AND DISCUSSION

The interaction between adsorbed hydrogen molecular on surface Si/Ge film and nanotube is investigated by using the first-principles calculation. Si/Ge nanotube is a new form of Si/Ge made by rolling up a single Si/Ge sheet, so narrow tube opened at both ends.

It is found that the binding energy of the physisorbed H_2 on Si/Ge nanofilm surface is weak, and it can increase significantly in a nanotube. The character of the binding dramatically changes when passing molecular H_2 functionalizes through it. Out of two adsorbed H_2, the first one can be adsorbed dissociatively and the second one is chemisorbed molecularly. The nature of binding has a very weak physisorption in the third adsorbed H_2. The Si/Ge, also, promotes the chemisorptions of H_2 with smaller binding energy. The present results reveal the important effect of passing the molecular H_2 through nanotube. These results will increase our understanding of the molecular and dissociative adsorption of hydrogen.

Simulations are run with the H_2 bond length at 0.75 Å, which is the optimum bond length of free H_2. Simulations are, also, run with the bond length at 1.16 Å, the optimized structure of H_2 attached to Si/Ge surface. The H-H interaction when absorbed on the surface is weakened, and; therefore, the H-H distance has increased to 1.16 Å.

The total binding energies, E_T, are obtained form the expression:

$$E_T = E_T[H_2] + E_T[Si/Ge] - E_T[H_2 + Si/Ge] \tag{12}$$

The total energies of free or absorbed H_2 on the Si/Ge nanofilm and Si/Ge nanotube, is at the same distance. The binding energies for both free H_2, ($E_T[H_2]$) and absorbed H_2, ($E_T[H_2 + Si/Ge]$) are considered at the lowest ground state of the total energies (either magnetic or non-magnetic); a bare Si/Ge surface has a non-magnetic ground state with zero net spin. $E_T > 0$, corresponds to optimized stable structure and indicates the bonding.

The molecular dynamics method is useful for calculating the time-dependent properties of an isolated molecule. However; more often, one of these properties of a molecule is interacting with other molecules. With HyperChem 7.0 program package [13], we can add H_2 molecules into the simulation explicitly, but the addition of many molecules will make the simulation much slower. A faster solution is to simulate the motion of the molecule of interest using Langevin dynamics and Monte Carlo simulation. To integrate the Langevin equations (2, 3), HyperChem uses the method [16] in calculation.

Both simulations were at different temperatures; the time step and friction coefficient for the Langevin simulation were 10^{-6} ps and 0.1 ps^{-1}, respectively [21, 22]. Monte Carlo simulations are commonly used to compute the average thermodynamic properties of a molecule or a system of molecules, and have been employed extensively in the study of the structure and equilibrium properties of molecules [14]. Monte Carlo calculations are similar to the molecular (or Langevin) dynamics calculations (discussed previously). Monte Carlo simulations employ a statistical sampling technique to generate configurations, which represent a trajectory in phase space. Thus, unlike molecular dynamics or Langevin dynamics, which calculate ensemble averages by calculating averages over time, Monte Carlo calculations evaluate the averages of the ensemble directly by sampling configurations from the statistical ensemble. If the run takes enough time, Monte Carlo and molecular dynamics must give the same average results for the same system. However, only molecular dynamics can calculate time-dependent properties of a system, such as rotational frequencies or transitional rates. On the other hand, Monte Carlo is generally better in sampling the allowed states of a system, and; thus, can often calculate the average properties more quickly and accurately (Figures 2, 3) when the temperature is increased the total energy is increased too. Therefore, the bonding distance is 1.16 Å, the total energy began to increase in low temperatures, which the total energy is stable in LD method and irregular in MC method when the temperature is high.
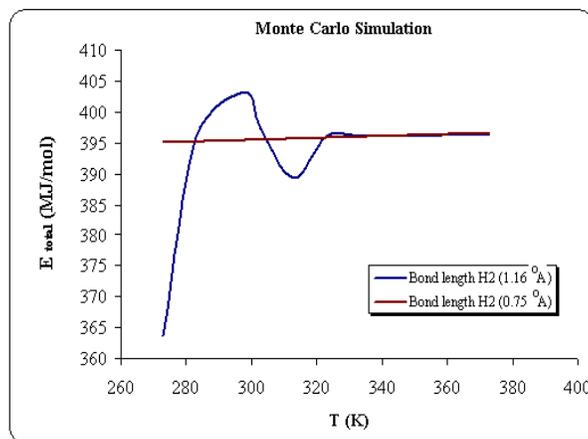
Figure 2. The total energy (MJ/mol) calculated for adsorption H_2 with different bond lengths on surface of Si-Ge film by Monte Carlo Simulation.
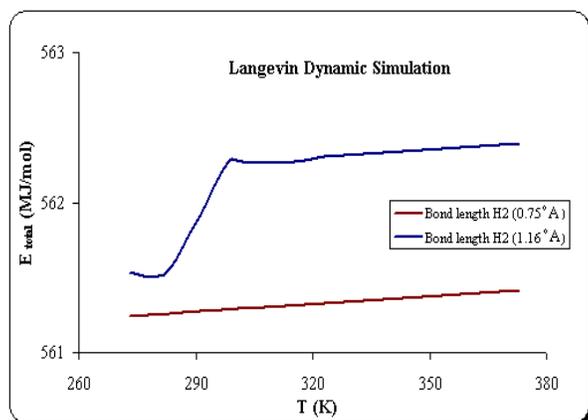

Figure 3. The total energy (MJ/mol) calculated for adsorption H_2 with different bond lengths on surface of Si-Ge film by Langevin dynamic simulation.

Table 1. The total energy, potential energy and kinetic energy (MJ/mol) calculated for adsorption of H_2 with different bond length on surface of Si/Ge film by Monte Carlo and Langevin daynamic simulation.

T (K)	Monte Carlo						Langevin dynamic					
	Bond length H_2 (0.75 Å)			Bond length H_2 (1.16 Å)			Bond length H_2 (0.75 Å)			Bond length H_2 (1.16 Å)		
	E_{Total}	E_{Pot}	E_{Kin}	E_{Total}	E_{Pot}	E_{Kin}	E_{Total}	E_{Pot}	E_{Kin}	E_{Total}	E_{Pot}	E_{Kin}
273	392.80	392.31	0.49	363.61	363.14	0.48	561.24	328.77	232.47	561.53	329.20	232.33
298	395.93	395.40	0.53	403.15	402.63	0.52	561.28	328.75	232.53	562.27	329.07	233.20
313	396.40	395.84	0.56	389.37	388.82	0.55	561.31	328.74	232.57	562.27	329.07	233.20
323	397.12	396.55	0.57	396.08	395.51	0.57	561.33	328.74	232.59	562.31	329.07	233.24
333	397.24	396.65	0.59	396.06	395.48	0.58	561.34	328.73	232.61	562.33	329.07	233.26
343	397.75	397.14	0.61	396.04	395.44	0.60	561.36	328.73	232.64	562.35	329.06	233.28
353	395.68	395.06	0.63	396.17	395.55	0.62	561.38	328.72	232.66	562.36	329.06	233.30
363	395.64	395.00	0.65	396.35	395.71	0.64	561.40	328.72	232.68	562.38	329.06	233.32

The results show which the interaction between H_2 and surface of Si/Ge nanofilm is endothermic. In Table 1, the total energy, potential energy and kinetic energy are calculated by Monte Carlo and Langevin dynamic simulation. Therefore, we tried to investigate the continued of converting surface Si/Ge nanofilm to nanotube. The molecular H_2 with bond lengths (0.75 and 1.16 Å) is passing through Si/Ge nanotube at various temperatures. The calculations are done by both methods (Tables 2 and 3). The results of both surfaces show which the binding energy for molecular H_2 interaction in Si/Ge nanotube is more increasing than in Si/Ge nanofilm. In nanotube, various charge locations are created in nanotube when the surface turned into nanotube. These locations are observed at 353 K in Figures 4 and 5.

Table.2. The total energy and kinetic energy (MJ/mol) calculated for across H_2 with bond lengths in Si/Ge nanotube by Monte Carlo simulation.

Distance Å	Bond length H_2 (0.75 Å)															
	273 K		298 K		313 K		323 K		333 K		343 K		353 K		363 K	
	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin
0	392.45	0.42	613.49	0.46	613.57	0.48	613.62	0.49	613.86	0.51	613.48	0.52	575.85	0.54	613.72	0.55
5.77	614.20	0.42	615.01	0.46	614.39	0.48	614.54	0.49	613.86	0.51	614.45	0.52	614.54	0.54	614.39	0.55
10.01	614.04	0.42	614.17	0.46	614.19	0.48	614.47	0.49	614.46	0.51	614.07	0.52	614.58	0.54	614.59	0.55
14.93	614.96	0.42	614.97	0.46	614.31	0.48	614.50	0.49	614.42	0.51	614.49	0.52	614.64	0.54	614.65	0.55
19.82	614.19	0.42	615.13	0.46	614.24	0.48	614.34	0.49	614.42	0.51	576.46	0.58	614.69	0.54	614.77	0.55
23.41	614.43	0.42	614.86	0.46	615.09	0.48	615.09	0.49	615.53	0.51	614.50	0.52	615.50	0.54	615.56	0.55
Distance Å	Bond length H_2 (1.16 Å)															
	273 K		298 K		313 K		323 K		333K		343 K		353 K		363 K	
	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin
0	575.46	0.42	615.32	0.46	615.11	0.48	615.10	0.49	615.36	0.51	615.30	0.52	615.41	0.54	615.52	0.55
5.77	614.50	0.42	614.37	0.46	613.93	0.48	614.31	0.49	614.36	0.51	614.27	0.52	614.42	0.54	614.79	0.55
10.01	614.92	0.42	615.27	0.46	614.78	0.48	615.47	0.49	575.37	0.51	615.42	0.52	615.51	0.54	615.55	0.55
14.93	614.86	0.42	615.08	0.46	613.99	0.48	614.29	0.49	614.16	0.51	614.36	0.52	615.07	0.54	614.99	0.55
19.82	615.27	0.42	615.32	0.46	615.35	0.48	614.97	0.49	615.38	0.51	614.72	0.54	614.72	0.54	614.67	0.55
23.41	614.68	0.42	614.87	0.46	615.25	0.48	614.21	0.49	614.29	0.51	614.84	0.54	614.84	0.54	614.61	0.55

Nanostructures have considerably higher surface areas than their bulk counterparts; therefore, the surfaces often play important, sometimes even dominant, roles in the nanostructure properties. Figures 4 and 5 show the variation of E_T for passing H_2 through Si/Ge nanotube at 353 K. For hydrogen with bond length of 0.75 Å, at first, the total energy increases when passing H_2 in the initial length of the nanotube, then it is stable to the end in Monte Carlo simulation. This process is not stable for hydrogen with 1.16 Å length by this method. Then in the middle of length the nanotube, it begins to increase again and at the end of it begins to decrease. The minimum value of the interaction E_T is 614.27 MJ/mol. In Langevin dynamic simulation method, the total energy begins to decrease in the initial length of the nanotube for H_2 with 0.75 Å bond length.

But the passing H_2 with 1.16 Å bond length, in this method, increases in the initial length, and; then, it decreases at the end length of nanotube Figure 5. The total energy and kinetic energy (MJ/mol) are calculated for passing H_2 with bond length 0.75 Å and 1.16 Å through Si/Ge nanotube by both methods Tables 2 and 3.

Table.3. The total energy and kinetic energy (MJ/mol) calculated for across H_2 with bond lengths in Si/Ge nanotube by Langevin dynamic simulation.

Distance Å	Bond length H_2 (0.75 Å)															
	273 K		298 K		313 K		323 K		333 K		343 K		353 K		363 K	
	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin
0	656.64	71.24	656.65	71.26	657.36	71.38	657.37	71.40	657.39	71.42	657.40	71.44	657.42	71.45	657.43	71.47
5.77	644.01	68.31	656.77	71.44	657.47	71.56	657.49	71.58	396.90	16.18	396.88	16.20	396.89	16.22	396.91	16.24
10.01	656.75	71.41	656.77	71.43	657.47	71.55	657.49	71.57	657.50	71.59	657.52	71.60	657.53	71.62	657.55	71.64
14.93	656.75	71.42	656.77	71.43	657.47	71.56	657.49	71.58	657.50	71.59	657.52	71.61	657.53	71.63	657.55	71.65
19.82	656.76	71.42	656.77	71.44	657.47	71.56	657.49	71.58	657.50	71.60	657.52	71.61	657.53	71.63	657.55	71.65
23.41	656.72	71.35	656.74	71.37	657.44	71.50	657.46	71.51	657.47	71.53	657.49	71.55	657.50	71.57	657.52	71.58
Distance Å	Bond length H_2 (1.16 Å)															
	273 K		298 K		313 K		323 K		333 K		343 K		353 K		363 K	
	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin	E total	E kin
0	657.84	71.68	657.69	71.47	657.71	71.50	657.73	71.52	657.74	71.53	657.76	71.55	657.77	71.57	657.79	71.59
5.77	657.94	71.88	657.79	71.67	657.81	71.69	657.83	71.71	657.74	71.53	657.86	71.75	657.87	71.76	657.89	71.78
10.01	657.75	71.57	657.79	71.62	657.81	71.64	657.83	71.66	657.84	71.68	657.86	71.70	657.87	71.71	657.89	71.73
14.93	657.75	71.61	657.79	71.66	657.81	71.69	657.83	71.70	657.84	71.72	657.86	71.74	657.87	71.76	657.89	71.78
19.82	657.75	71.58	657.79	71.63	657.82	71.65	657.83	71.67	657.85	71.69	657.86	71.70	657.88	71.72	657.89	71.74
23.41	657.67	71.49	657.71	71.54	657.73	71.57	657.75	71.58	657.76	71.60	657.78	71.62	657.79	71.64	657.81	71.66
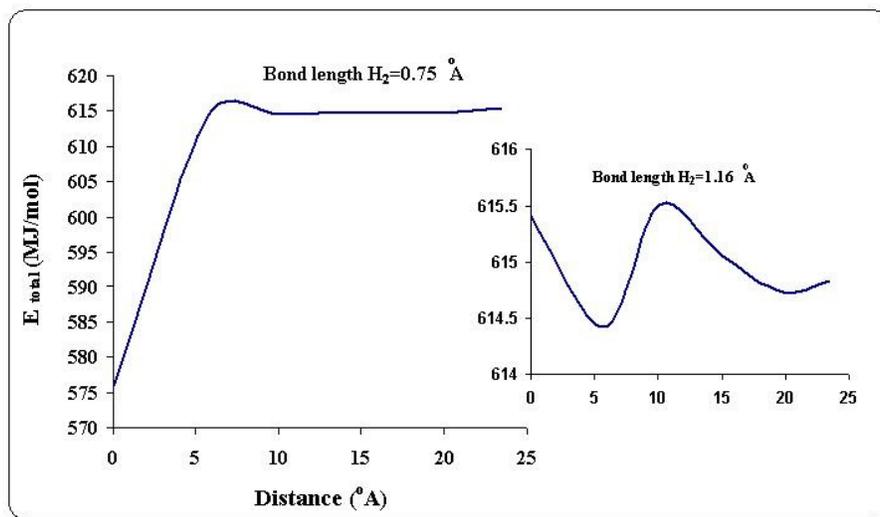
Figure 4. The total energy (MJ/mol) calculated for across H_2 with bond lengths in Si/Ge nanotube by Monte Carlo Simulation at 353 K.
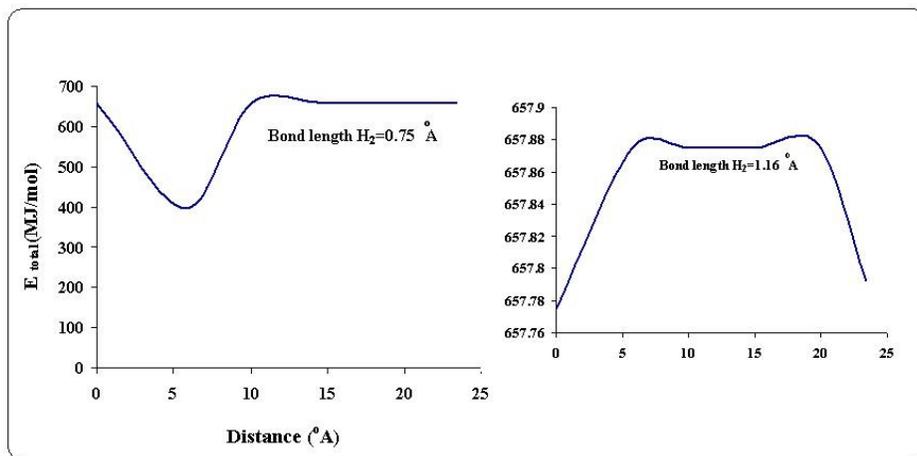
Figure 5. The total energy total (MJ/mol) calculated for across H_2 with bond lengths in Si/Ge nanotube by Langevin dynamic simulation at 353 K.

CONCLUSION

In this work, we present a detailed analysis of the interaction between hydrogen molecules on the surface of Si/Ge nanofilm and by passing H_2 through Si/Ge nanotube at different temperatures. These calculations are done by Monte Carlo and Langevin dynamic simulation in HyperChem 7.0 package program. In general, Langevin dynamics simulations are the same as molecular dynamics simulations. There are differences due to the presence of additional forces. Most of the earlier discussions on simulation parameters and strategies for molecular dynamics had been applied to Langevin dynamics.

We found that the binding energy between H_2 molecule and outer surface of a bare Si/Ge is very weak and the physisorption bond can easily be broken. The H-H interaction when absorbed on the surface is weakened, and; therefore, the H-H distance has increased to 1.16 Å. The results have shown that the bond in the molecular interaction of H_2 is relatively stronger with a shorter bond length, so energy changes are regular when passing H_2 through nanotube. The binding energy would increase if H_2 molecule was directly attached to Si/Ge surface. However, the case with the Si/Ge atom leads to a relative weaker interaction and smaller binding energies. MC and LD simulation were run for the interaction H_2 and the surface results in a kind of binding between chemisorptions and physisorptions the binding energy. In this case, the H-H bond length is stretched a bit from the normal value 0.75 to 1.16 Å. When the temperature is increased, the total energy, kinetic and potential energy are enhanced, so this interaction is endothermic. The calculated energy for the two systems shows that nanotube has considerably higher surface areas than their most counterparts.

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