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Tight-binding potential for hydrocarbons

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A new tight-binding potential model for hydrocarbons is developed based on a previous carbon tight-binding model. The features of this interesting model have been examined using a variety of configurations of hydrocarbons. The resulting geometries, energetics of small hydrocarbon molecules and hydrogenated diamond surfaces, are in qualitative agreement with previous results. The model especially describes well the abstraction of one hydrogen atom from either a methane or hydrogenated diamond (100)(2×1) surface by the vapor H radical. The kinetic behavior of polymerization reactions is correctly predicted too.

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I. INTRODUCTION

Atomistic computer simulation has become a powerful tool in our understanding of complicated matter. Nowadays, computer power increases rapidly, enabling us to simulate more complex systems than before. On the other hand, scientists develop theoretical methods and efficient algorithms in an attempt to deal with large complicated systems. For example, developing $O(N)$ algorithms[1] and generating tight-binding (TB) potentials are attractive intensively. $O(N)$ method, which is characterized with linear scaling with respect to the size of a system, is a promising tool for the large-scale calculations of the electronic structures of huge systems. The TB method, as we know, offers a good compromise between the first-principle techniques, which are more accurate but much more costly, and empirical potentials, which are cheaper to use but often not transferable to configurations being different from the fitted. Therefore people can simulate some large complicated systems to get insight into concerned physical properties by using transferable TB methods.

There are many TB potentials developed so far, and numerous significant results have been obtained within the scheme of the TB method.[2] However, as we know, the transferability of any developed TB potential is limited to some extent, because the on site and intersite terms as well as repulsive potential in the TB formalism are parametrized simply, also the basis set is minimal usually, and the fitting procedure is artistic. Until now, generating TB potential with high quality has been a challenging task.

Recently, developing TB potential models is not only focused on systems consisting of one kind of element, but also extended to some binary systems such as SiC,[3] GaN,[4] SiH,[5] CH,[6–9] and so on. Especially, for hydrocarbon TB model, we noted that Devidson and Pickett reported[6] their TB potential based on the TB parameters for the C-C interactions given in Ref. 10. This set of TB parameters shows a good result on hydrogenated diamond surfaces. Later on, Horsfield *et al.*[9] proposed a different version of TB model for hydrocarbon by improving the version of Devidson and Pickett,[6] from which most of the tested results are in excellent agreement with experimental values or accurate *ab initio* results except for the kinetic behavior of polymerization reactions.[11] More recently, Tuyarot *et al.*[12] have employed this modified TB model to compute the energies, structures, and elastic properties of polyacetylene isomers; they found that the resulting geometries and Young's moduli of the polyacetylene isomers are in excellent agreement with those from previous *ab initio* calculations, whereas some electronic-structure-related properties of the polyacetylene could not be described. Overall, the TB model from Horsfield *et al.*[9] has a good transferability, which is available for realistic research although there are limitations in it as mentioned above. Basically, the limitations of this model are originated from the transferability of interactions of C-C, C-H, and (or) H-H. Thus enhancing the transferability of a TB model for hydrocarbon means to improve the transferability of the three kinds of interactions. We noted that for the interactions of C-C, an environment-dependent TB potential has been proposed more recently.[13] The correction of environment dependent in this TB model for carbon is achieved by introducing rescaled distance between atoms and a screening factor into the matrix elements and pairwise interaction. Either of the rescaled distance and the screening factor are the function of the number of atoms which are located within overlap cutoff range of two interacting atoms. The more the number of the atoms within the overlap range is, the weaker the interaction between the two atoms is. The transferability of this interesting carbon TB model was demonstrated to be better than that[10] employed in the above two TB potentials.

On the other hand, investigating reactions during the growth of diamond films as well as the interaction between free polymerization radicals is also paid much attention. As we know, the processes of the reactions are governed by the kinetic behavior. On the theoretical side, it is significant to develop a TB model to correctly describe kinetic behavior of some reactions. For this purpose, we develop a version of TB model for hydrocarbons (CHTB) based on the environment-dependent TB model of carbon.[13] Our results show that this CHTB can describe the structures and energies of many different hydrocarbons as well as energy barriers of some typical reactions.

II. METHOD

In tight-binding approximation, the Hamiltonian is given by

TABLE I. The parameters for C-H and H-H. α_1 is in eV, the others are dimensionless.

	α_1	α_2	α_3	α_4	r_c	w_d
$ss\sigma$ (C-H)	-6.0507	0.07895	0.06860	3.89720	1.62	0.08
$sp\sigma$ (C-H)	6.1105	0.00458	0.02860	3.08320	1.62	0.10
ϕ (C-H)	12.00271	0.28742	0.34878	0.90000	1.5828	0.07649
$ss\sigma$ (H-H)	-4.97593	0.60000	0.39830	6.00000	0.98	0.082
ϕ (H-H)	4.10159	1.80000	1.20580	1.17483	0.98	0.042

$$H_{TB}=\sum_{i,\alpha}\varepsilon^{i}_{\alpha}a^{+}_{i,\alpha}a_{i,\alpha}+\sum_{i,j,\alpha,\beta}v^{i,j}_{\alpha,\beta}(r_{i,j})a^{+}_{i,\alpha}a_{j,\beta}. \tag{1}$$

Here, α and β stand for the atomic orbitals, and i,j for the labels of the atoms. ε^{i}_{α} is atomic orbital energy of orbital α in atom i, $v^{i,j}_{\alpha,\beta}$ is the hopping parameters between atomic orbital α of atom i and atomic orbital β of atom j. As usual, $2s$ and $2p$ orbitals for carbon and $1s$ orbitals for hydrogen atoms are taken into account in this TB model.

The total energy is written as

$$E_{tot}=E_{bs}+E_{rep}, \tag{2}$$

where the band structure energy $E_{bs}=\Sigma^{occ}_{k}n_k\varepsilon_k$, and the repulsive energy is expressed as a function as below,

$$E_{rep}=\sum_{i} f\left(\sum_{j}\phi(r_{i,j})\right), \tag{3}$$

where $\phi(r_{i,j})$ is a pairwise potential for atoms i and j, and f is a functional expression of polynomial, ε_k is the eigenvalue of the kth energy level. n_k is occupation number in energy level k.

Generally, the bonding characters of C-C, C-H, and H-H in a complicated hydrocarbon system are different from one another, which can be roughly characterized by different coordination numbers of C or H. For carbon, Tang *et al.*[10] reported that the bonding environment correction does strikingly improve the fitting energy band structures and cohesive energy curves for the various phases that are characterized by different coordination numbers such as 2,3,4,6,8, and 12, totally. However, owing to the fact that the coordination number of H atoms are no more than 2, predominantly are 1, we thus believe that the interaction between C and H is much localized as well as monotonous so that the bonding environment correction nearby a bonded H atom is not so important. As a consequence, we utilize simple formulas without cor-

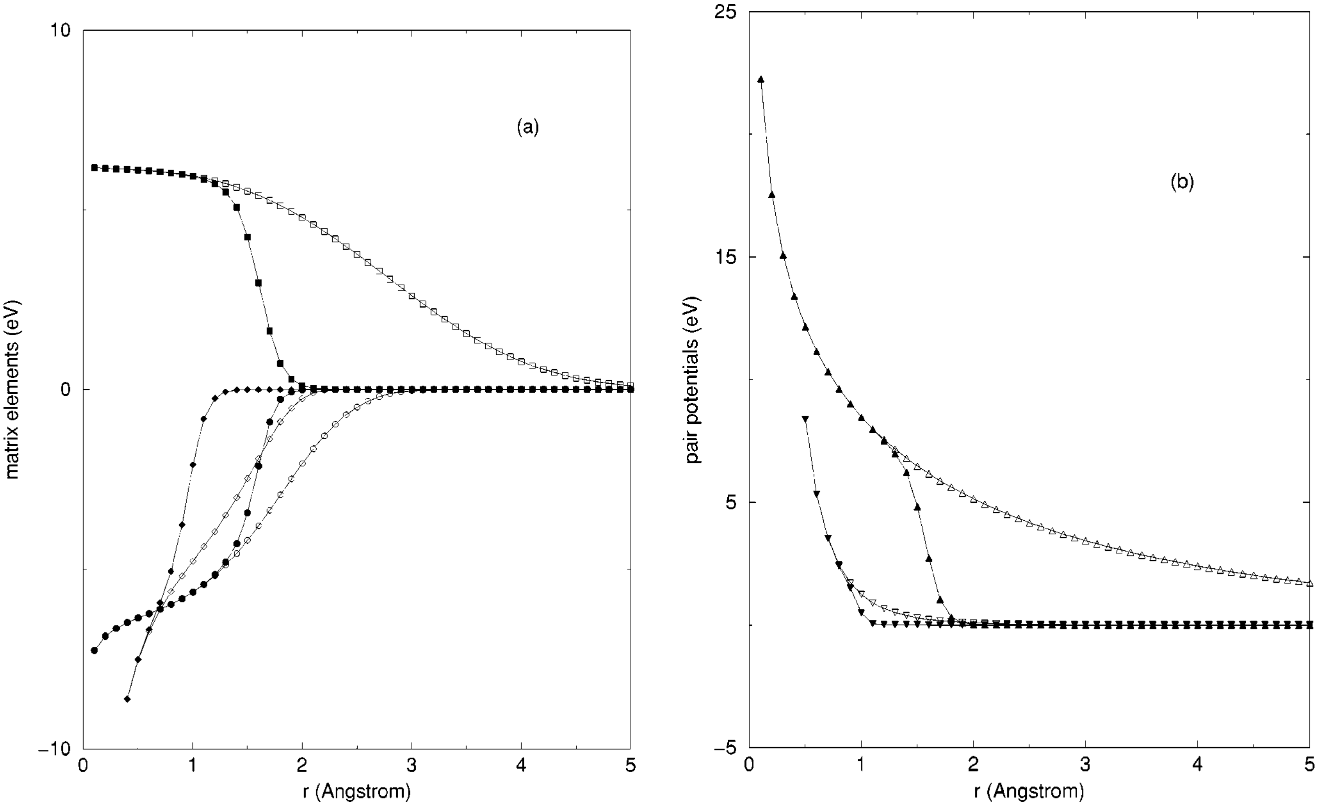

FIG. 1. Matrix elements of $h^{C-H}_{ss\sigma}(r)$ (circle), $h^{C-H}_{sp\sigma}(r)$ (square) and $h^{H-H}_{ss\sigma}(r)$ (diamond) in panel (a), and pair potentials of $\phi(r)^{C-H}$ (triangle up) and $\phi(r)^{H-H}$ (triangle down) in panel (b). The solid symbols stand for the cases appended by cutoff function, and the hollow ones for the cases with $f_c=1$.

TABLE II. The coefficients of the polynomial function.

	c_0 (eV)	c_1 (eV^{-1})	c_2 (eV^{-2})
(C-H)	0.00001	0.54437	-0.00298
(H-H)	0.001	0.60000	0.001

rection of bonding environment around a H atom to express the interactions of C-H and H-H.

In detail, the formulas together with related parameters of on site, hopping terms and pairwise potential for pure carbon systems are adopted from Ref. 13. The on site terms corresponding to hydrogen are set simply equal to the atomic orbital energy of hydrogen, E_s^H. The value of E_s^H is taken to be 1.5 eV. The hopping parameters and pairwise repulsive potential of either C-H or H-H interactions are expressed in a same form as below,

$$h(r_{ij}) = \alpha_1 r_{ij}^{-\alpha_2} \exp[-\alpha_3 r_{ij}^{\alpha_4}] f_c . \tag{4}$$

Here, the cutoff function

$$f_c = \{1 + \exp[(r_{ij} - r_c)/w_d]\}^{-1}. \tag{5}$$

r_{ij} denotes the distance between atoms i and j, $\alpha_k (k = 1,2,3,4)$, r_c and w_d are parameters determined through fitting. The role of f_c in Eq. (4) is to truncate the interactions between atom i and j in a smooth manner. In the expression of repulsive energy above, the polynomial f of second order for C-H and H-H is used in this model.

The parameters in this model are obtained through fitting to LDA (local-density approximation) results (i.e., energy levels and cohesive energies) of small hydrocarbon molecules, the obtained parameters are summarized in Table I. In order to show the effect of the cutoff function in Eq. (4), we, based on Eq. (4) and the related parameters in Tables I and II, calculated the distance dependence of hopping matrix elements and pair functions for both C-H and H-H, as well as the distance dependence when $f_c = 1$, as shown in Fig. 1. Clearly, in comparison with the cases without cutoff function, the amplitudes of the hopping matrix elements and pair function appended with cutoff function decay rapidly when $r \leqslant 1.9$ Å for C-H, and nearly vanish when $r \leqslant 1.3$ Å for H-H. As a consequence, the cutoff functions used here do effectively shorten the interaction range between atoms. These allow us to take 1.9 Å as the cutoff for C-H, and 1.3 Å as the cutoff for H-H in this model, reasonably.

To perform molecular-dynamics simulation using the TB model, it is necessary to obtain the attractive forces and repulsive forces on atoms. The former is obtained according to the Hellmann-Feynman theorem, and the latter is directly the gradient of E_{rep}.

III. RESULTS

In order to reveal the properties of the generated model as described in Sec. II, we chose molecules, surfaces, and bulk for test. In the following calculations, there is no periodic condition imposed for molecular systems, but the periodic conditions are applied for surfaces and bulks. In addition, we employ supercells to mimic the surface systems and the bulks concerned, the point $k = 0$ of the reciprocal lattice is thus taken into account only.

We begin with we test for some small hydrocarbons, such as CH, CH_2, CH_3, CH_4, C_2H_2, C_2H_4, C_2H_6, and C_6H_6. All of these molecules are fully relaxed. Tables III and IV, respectively, list the calculated bond lengths, bond angles, and cohesive energies of the selected molecules together with related experimental values. Our calculated bond lengths and bond angles of these molecules are in excellent agreement with those from experiment,[14] and the calculated energies are also consistent with experimental ones.[15]

Consequently, it is important to examine the features of this model in estimation of barriers for some typical reactions, for example, the reactions between radicals, hydrogen and radicals, hydrogen and diamond surfaces. One of the

TABLE III. A comparison of bond lengths (in Å) and related bond angles (in degree) of hydrocarbons from present calculations with those from previous theoretical calculations and experiment.

	This work	TB (Ref. 9)	TB (Ref. 7)	Experiment (Ref. 14)
CH	1.17(CH)		1.138(CH)	1.12(CH)
CH_2	1.16(CH)		1.134(CH)	1.11(CH)
	99.1(HCH)		98.6(HCH)	102.4(HCH)
CH_3	1.10(CH)		1.114(CH)	1.08(CH)
	120.0(HCH)		116.8(HCH)	120.0(HCH)
CH_4	1.10(CH)	1.09(CH)	1.116(CH)	1.09(CH)
C_2H_2	1.09(CH), 1.20(CC)	1.23(CC)	1.099(CH), 1.206(CC)	1.06(C-H), 1.207(C-C)
C_2H_4	1.16(CH), 1.30(CC)	1.077(CH), 1.338(CC)	1.113(CH), 1.321(CC)	1.08(CH), 1.33(CC)
	120.5(CCH)	121.0(CCH)	116.3(CCH)	121.4(CCH)
	119.3(HCH)	117.8(HCH)		117.8(HCH)
C_2H_6	1.19(CH), 1.44(CC)		1.119(CH), 1.503(CC)	1.09(CH), 1.526(CC)
	109.8(CCH)			110.9(CCH)
	109.1(HCH)		108.0(HCH)	107.4(HCH)
C_6H_6	1.13(CH), 1.37(CC)		1.114(CH), 1.389(CC)	1.09(CH), 1.397(CC)

TABLE IV. Atomization energies of selected hydrocarbons. The energies are in eV/atom.

	This work	TB (Ref. 9)	TB (Ref. 7)	Experiment (Ref. 15)
CH_4	-3.45	-3.52	-3.52	-3.52
C_2H_2	-3.98		-4.38	-4.08
C_2H_4	-3.85	-3.93	-3.99	-3.93
C_2H_6	-3.79	-3.75	-3.81	-3.71
C_6H_6	-4.81	-4.79	-4.97	-4.79

typical reactions between hydrogen and hydrocarbons is

$$CH_4+H\rightarrow H_3C-H-H\rightarrow CH_3+H_2. \qquad (6)$$

It was experimentally revealed that there is an energy barrier of 0.52 eV in the above reaction.[16] On the theoretical side, simulated by using *ab initio* methods, the theoretical energy threshold of the reaction (6) along the reaction coordinate with C_{3v} symmetry was estimated to be around 0.58 eV.[17] Following the previous calculation, we obtained an energy barrier of 0.61 eV for the reaction (6) using the present TB model. Our calculated value of energy barrier is slightly higher than the experimental result, yet comparable to the value of 0.58 eV from *ab initio* calculation. From our calculation, the barrier along the linear reaction coordinate is at a carbon hydrogen bond length of 1.51 Å and a hydrogen hydrogen bond length of 0.73 Å, closer and shorter than the *ab initio* results[17] of 1.47 and 0.93 Å, respectively.

Similar to Ref. 11, we also calculated polymerization reaction as shown in Fig. 2. Initially, the geometries of C_2H_4 and C_2H_5 radicals are separate each other as shown in Fig. 2(a), followed by approaching atom 3 towards atom 2 [labeled in Fig. 2(a)] step by step to mimic the reaction between C_2H_4 and C_2H_5. In each step, we fixed the positions of atom 2 and atom 3, and relaxed the rest of the atoms. The two reactants, C_2H_4 and C_2H_5, will interact with one another when the distance between the two carbon atoms (2 and 3) is less than the cutoff value of C-C. The final geometry shown in Fig. 2(b) is obtained through full relaxation. We found that there is an energy barrier of 0.4 eV in this reaction, which is close to experimental values ranging from 0.25 to 0.36 eV.[18]

Another test of this model is to check the accuracy of the interaction between hydrogen and diamond surfaces. We selected a slab model to mimic the clean diamond (100)(2×1) surface with respect to the chemical vapor deposition (CVD) diamond film growth. The slab used here consists of 12 atomic layers with 384 carbon atoms, the two surfaces in a slab are identical due to the inversion symmetry in it. All of the atoms in the slabs are allowed to be relaxed until the largest force on an atom is less than 0.01 eV/Å. After relaxing, we found that the basic feature in the diamond (100) (2×1) surface is symmetric dimer reconstruction. The bond length of dimers and spacings between different atomic layers in the clean surface are consistent with those from *ab initio* calculations,[19,20] as listed in Table V. In particular, our calculations also show that there are bucklings in the third and forth interlayer spacings. The bucklings in both spacings are found to be 0.20 and 0.04 Å, respectively, in which, as compared with literature,[20] the value of the former is much closer to the buckling of 0.26 Å from LDA calculation, and the latter is yet much lower than the LDA value of 0.16 Å. To go further, the above clean reconstruction is covered with a monolayer of hydrogen atoms. After full relaxation, we found that the main feature of the hydrogen-terminated surface also matches the LDA results[19,20] and LEED (low-energy electron diffraction) measurement[21] well, as summarized in Table VI. Notably, LEED results[21] indicated that the second interlayer spacing in the hydrogenated diamond (100)(2×1) surface is 0.96 Å with 0.06 Å error. This, in other words, corresponds to a 3.4% expansion relative to the bulk spacing. Clearly, the LDA results listed in Table VI cannot describe such expansion, yet the calculated interlayer spacing from present model accords with the results from LEED measurement[21] very well. In addition, the buckling with 0.18 Å in the third interlayer spacing was found too,

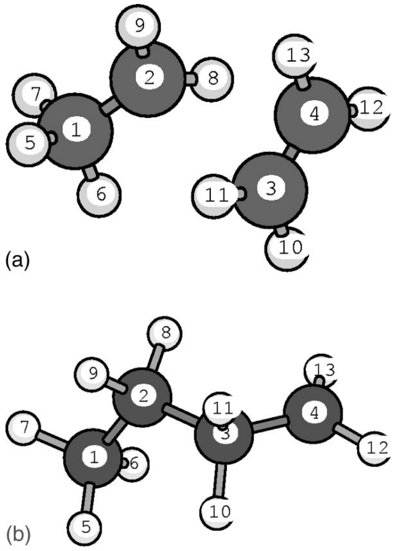

FIG. 2. The reaction for the polymerization of ethene. (a) Initial geometry, (b) final geometry.

TABLE V. A comparison of results from calculations for clean diamond (100)(2×1) reconstruction. l_{C-C} is the dimer bond length of carbon atoms in surface, Δ stands for the change of the spacing between concerned atomic layers relative to the value of bulk-terminated structure.

	This work	TB (Ref. 9)	TB (Ref. 6)	LDA (Ref. 19)	LDA (Ref. 20)
l_{C-C} (Å)	1.342	1.398	1.398	1.40	1.37
Δ_{12} (%)	-21.0	-25.4	-24.8	-24.0	-24.0
Δ_{23} (%)	$+1.0$	$+7.2$	$+8.26$	$+3.0$	$+3.0$

TABLE VI. A comparison of results from calculations and experiment for H terminated diamond (100) $\times(2\times1)$ reconstruction. l_{C-C} and l_{C-H} are the dimer bond length of carbon atoms in surface and the bond length between carbon atom and hydrogen atoms, respectively. Δ stands for the change of the spacing between concerned atomic layers relative to the value of bulk-terminated structure.

	This work	TB (Ref. 9)	TB (Ref. 6)	LDA (Ref. 19)	LDA (Ref. 20)	Expt. (Ref. 21)
l_{C-C} (Å)	1.57	1.62	1.62	1.67	1.61	1.55–1.65
l_{C-H} (Å)	1.06	1.09	1.12	1.17	1.01	
Δ_{12} (%)	-12.0	-8.20	-9.24	-3.0	-9.0	-7
Δ_{23} (%)	$+1.1$	$+0.7$	$+12.71$	-0.3	-0.2	3.4

which is in excellent agreement with the value of 0.19 Å from LDA calculation. We furthermore considered an abstraction of a hydrogen atom from the hydrogenated diamond (100)(2×1) surface. Our calculation shows that this reaction is endothermic, with reaction energy of 2.9 eV, being lower than the LDA result of 4.18 eV.[22] We also estimated the reaction energy when a H atom is abstracted from the monohydride dimer of diamond (100)(2×1) surface by the vapor H radical, the reaction energy of 0.10 eV is predicted based on our calculations, being higher slightly than the reaction energy of 0.04 eV from LDA calculations.[22]

Finally, the formation energy of one hydrogen atom as an interstitial impurity in crystalline diamond has been carried out in supercell approximation. The supercell contains 64 carbon atoms and a single hydrogen atom. The hydrogen atom is located at three typical sites within the crystalline, i.e., *T* (tetrahedral), AB (antibonding site lying in direction opposite to a C-C bond), and BC (bond center) sites. Taking the cohesive energy of configuration with *T* site as a reference, the relative cohesive energies of BC and AB sites are -0.50 and 0.03 eV, respectively, implying that configuration with the BC site is more stable than the others. Previously, several groups[23–25] have calculated the relative cohesive energies of BC in an approximation of clusters by using ab initio calculations, the predicted relative energies of BC site range from -2.7 to -0.95 eV, among which the value of -0.95 eV is the latest. So, the relative cohesive energy of BC configuration from our calculation is underestimated. After examining the geometry of BC configuration, we found that the hydrogen atom at the BC site causes an elongation of the C-C bond by 46% from our calculations, being consistent with the value of 50% from previous calculation using a local spin-density approximation.[26]

IV. SUMMARY

In conclusion, we have developed a tight-binding model for hydrocarbons based on a previous carbon tight-binding model. The present model predicts the energies and structures of small hydrocarbon molecules, hydrogen atoms as an interstitial impurity within bulk diamond, and hydrogenated diamond (100)(2×1) surface correctly. These predictions together with the excellent agreement of energy barriers of some typical reactions with previous results demonstrate that this model has a good transferability. We anticipate that this potential model will be useful for the molecular-dynamics simulation studies of the growth of synthetic diamond films.

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