

Neural network correction for heats of formation with a larger experimental training set and new descriptors

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Received 21 March 2005; in final form 12 May 2005

Available online 13 June 2005

Abstract

A neural-network-based approach was applied to correct the systematic deviations of the calculated heats of formation for 180 organic molecules and led to greatly improved calculation results compared to the first-principles methods [J. Chem. Phys. 119 (2003) 11501]. In this work, this neural network approach has been improved by using new descriptors obtained from natural bond orbital analysis and an enlarged training set including organic, inorganic molecules and radicals. After the neural network correction, the root-mean-square deviations for the enlarged set decreases from 11.2, 15.2, 327.1 to 4.4, 3.5, 9.5 kcal/mol for the B3LYP/6-31G(d), B3LYP/6-311G(2d,d,p) and HF/6-31G(d) methods, respectively.

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1. Introduction

In the past few decades, important theoretical insights have led to the development of sophisticated and accurate theoretical techniques that can now be applied to a variety of problems of chemical interest. These theoretical methods include configuration interaction (CI), coupled-cluster (CC) theory, and the Gaussian 2 (G2) [1–3], Gaussian 3 (G3) [4–6] algorithms and so on. However, these procedures are most computational resource consuming and are still inapplicable to complex systems. Density-functional theory (DFT), especially hybrid methods such as B3LYP [7–10], surely offers a promising alternative. However, the errors of DFT calculations are accumulated with the size of the molecules [11] because of employing the approximated exchange-

correlation (XC) functional. Thus, a balance has to be found between accuracy and efficiency.

Neural network (NN) approaches have become popular in chemistry and physics during the last 10 years [12,13], because of their ease of use and their wide applicability to standard problems. Particularly, in chemical physics, NNs have been recently applied with great success. For example, NNs have been used to calculate the ground state eigenenergy of two-dimensional harmonic oscillators [14], to obtain the electronic correlation energy for atoms and diatomic molecules [15], to predict oxidation energies [16], and to model localized electron pair correlation energies [17]. Recently, Chen et al. [18,19] have developed a combined first principle calculation and neural network correction approach to improve significantly the accuracy of the calculated thermo-chemical properties. The physical descriptors employed in their work were the calculated ΔH_f^0 , the total number of atoms in the molecules (N_t), zero-point vibrational energy (ZPE), and the number of double

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bonds (N_{db}) or the number of hydrogen atom in a molecule (N_H). The systematic deviations between the calculated ΔH_f^0 and experimental measurements were eliminated greatly. For the 180 small- to medium-sized organic molecules, the root-mean-square (RMS) deviations of the calculated heats of formation were reduced from 21.4 to 3.1 kcal/mol and from 12.0 to 3.3 kcal/mol after the NNs correction was applied for the B3LYP/6-311 + G(d,p) and B3LYP/6-311 + G(3df,2p) methods, respectively [18].

We have also developed a linear regression correction (LRC) approach using electron numbers in different chemical environment as descriptors to successfully correct the unbalanced electron correlation energy theoretically calculated between a molecule and its composing atoms [20,21]. Although LRC approach is mathematically more straightforward, its results are usually inferior to the NN correction approaches using the same physical descriptors. In addition, Allinger and coworkers [22,23] also developed a different approach, in which, the bond/group equivalents, number of bonds, and other descriptors were used to empirically correct the HF or DFT electronic energies to obtain heats of formation of organic molecules. Their results were very accurate, but it is difficult to apply their schemes to the molecules with irregular bonds.

Although very successful, the training set of the previous NN approaches contains only closed-shell organic molecules, which limits the application range of the method. Therefore, the training set including 350 heats of formation of small and medium-sized organic, inorganic molecules, and radicals used in [21] is employed in the present work. Furthermore, a new set of physical descriptors as employed in our previous LRC approaches [21], the electron populations of different type of natural bond orbitals (NBO) [24–28] are adopted in the current NN approach.

2. Computational methods

Geometry optimizations and vibrational frequency analyses were carried out at the B3LYP/6-31G(d), B3LYP/6-311G(2d,d,p) and HF/6-31G(d) levels of theories. The more balanced 6-311G(2d,d,p) basis set as employed in the modified complete basis set model (CBS-QB3) [29] is used in our present work, which includes two sets of d functions on elements beyond the first row, one set of d polarization functions on the first row elements, and one set of p polarization functions on hydrogen as well. Diffusion basis functions have not been tested here because they are expected to have a trivial effect on the molecules in our training set since they are all neutral. The calculation of ΔH_f^0 is based on an atomization energy scheme [30], in which the scale factors for the zero-point vibrational energies (ZPE)

are 0.9806, 0.9900 and 0.9135, and those for calculating the enthalpy change of a molecule from 0 to 298.15 K ($\Delta H_{298K}^{calc}(M)$) are 0.9989, 0.9900 and 0.8905 for the B3LYP/6-31G(d), B3LYP/6-311G(2d,d,p) and HF/6-31G(d) methods, respectively [31,29]. NBO analyses at corresponding theoretical level were carried out to evaluate the populations of the electrons, which were performed with NBO 3.1 as implemented in the GAUSSIAN 03 package of programs [32]. Attentions must be given to the NBO calculations for radicals and strongly delocalized molecules. For example, for radicals NO, ClO, CN, HCO, CH₃CO and H₂COH the SCHOOSE keyword is needed to specify the correct bonding pattern. For benzene and substituted benzene molecules the RESONANCE keyword should be used. All the calculations in the present study were performed with the GAUSSIAN 03 suite of programs [33].

3. The neural network approach

A three-layer architecture for the neural networks was adopted in the current approach, including an input layer consisting of inputs from the physical descriptors (x_1, x_2, \dots), a hidden layer containing two hidden neurons (y_1, y_2), and an output layer that outputs the corrected values for the property of interest (Fig. 1). $\{W_{x_{ij}}\}$ and $\{W_{y_j}\}$ are sets of the connection weights of the links. $\{W_{x_{ij}}\}$ connects the input neurons and the hidden neurons, and $\{W_{y_j}\}$ connects the hidden neurons and the output neurons. The form of the transfer function used in this neural network is tangent sigmoid function (TANSIG), and the output is calculated according to

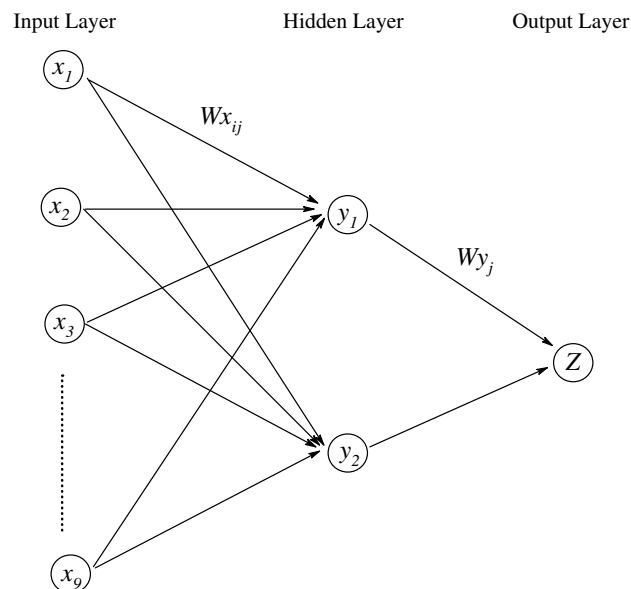


Fig. 1. The structure of the neural network.

$$Z = \sum_{j=1}^n W_{y_j} \text{Sig} \left(\sum_{i=1}^m W_{x_{ij}} X_i \right),$$

where $\text{Sig}(v) = 2/(1 + \exp(-2*v)) - 1$. The number of descriptors for the input layer is nine in this work. They are the total electron populations of different NBOs: 2-center bond (BD), 1-center core pair (CR), 1-center valence lone pair (LP), 1-center Rydberg (RY*), 2-center anti-bond (BD*), and valence non-Lewis lone pair (LP*). The core electrons are further divided into several subsets according to the shell in the corresponding atoms. We define CR1, CR2, and CR3 as the first, the second and the third layer below the valence shell. For a given molecule, the total CR1 is the sum of all CR1 of the composing atoms, and the same for CR2 and CR3. Taking CBrCl₃ as an example, the CR1 of C element is 2, the CR1 of Cl element is 8 and the CR2 is 2, and the CR1 of Br is 18, the CR2 is 8 and the CR3 is 2. Thus, for CBrCl₃, the CR1 is 44, the CR2 is 14, and the CR3 is 2. The number of the unpaired electrons of atom in the ground state is also included as a descriptor. The 350 molecules are randomly divided into the training set (300 molecules) and the testing set (50 molecules). In order to ensure the quality of our neural network and avoid over-fitting, a cross-validation procedure is employed. We further divide the 300 training molecules randomly into six subsets of equal size. Five of them are used to train the neural network, and the sixth to validate its predictions. This procedure is repeated six times in rotation.

4. Results and discussion

The corrected ΔH_f^0 s of the three methods compared to the experimental values are illustrated in Fig. 2a–c for the B3LYP/6-31G(d), B3LYP/6-311G(2d,d,p) and HF/6-31G(d) methods, respectively, in which the asterisks belong to the training set, the triangles belong to the validating set, and the crosses belong to the testing set. In comparison, the raw calculated ΔH_f^0 values are illustrated in Fig. 2d,e,f, respectively. The mean absolute deviation (MAD) and RMS deviation of the corrected results with their experimental counterparts are listed in Table 1. The weights $\{W_{x_{ij}}\}$ and $\{W_{y_j}\}$ are listed in Table 2.

The raw calculated results have very large systematic errors compared with the experimental results [23]. Upon the NN correction the deviations are all substantially decreased. For the B3LYP/6-31G(d) method, the MAD was reduced from 8.2 to 3.2 kcal/mol, and for the B3LYP/6-311G(2d,d,p) method, it was reduced from 12.4 to 2.3 kcal/mol. For the HF/6-31G(d) method, the MAD was dramatically reduced from 284.1 to 6.8 kcal/mol and decreased by more than 30 times. RMS deviation analysis further demonstrates that this NN correction approach greatly decrease the calculation

errors of the DFT and HF methods. For the B3LYP/6-31G(d) and B3LYP/6-311G(2d,d,p) methods, the RMS deviations were reduced from 11.2 to 4.4 kcal/mol and from 15.2 to 3.5 kcal/mol, respectively, and for the HF/6-31G(d) method, it was reduced from 327.1 to 9.5 kcal/mol. In the insets of Fig. 2a,b,d,e, the histograms for the deviations (from the experiments) are plotted, which further demonstrate that the NN correction approach greatly decreases the large systematic calculation errors of the DFT methods.

Truncation error in the basis set can be greatly corrected by the NN approach. The corrected results using the smaller 6-31G(d) basis set nearly have the same accuracy as those using the larger 6-311G(2d,d,p) basis set for the 350 molecules. Thus, smaller basis set can be used in the NN scheme to save a significant amount of computer time required for large molecules. Moreover, the deviations of large molecules are of the same magnitude as those of small molecules. Unlike most other calculations that yield worse results for large molecules than that for small ones, the NN approach does not discriminate against the large molecules [18]. For example, the deviations for C₁₀H₁₈O₄ and C₁₂H₁₀ before correction are 20.4 and 15.9 kcal/mol at the B3LYP/6-31G(d) level, respectively, while the deviations after the NN correction drop to 0.6 and 1.3 kcal/mol, respectively.

Compared to the LRC approaches using the same NBO descriptors, the results of NN approach are slightly better. Upon the linear regression correction, the RMS deviations for the 350 molecules are 4.5, 4.0 and 10.2 kcal/mol for the B3LYP/6-31G(d), B3LYP/6-311G(2d,d,p), and HF/6-31G(d) methods, respectively [21]. The reasons may be contributed from two facts: (1) The NN approach involves non-linear functions to correct the calculated data, but the linear regression method does not. (2) No matter the NNs or the LRC method, more adjustable variables usually give better results. It is known that each input descriptors has a certain relationship with each hidden neurons in the neural network. Thus, the present neural network architecture that adopts two neurons in the hidden layer should have more adjustable variables during the fitting process compared to the linear regression method, in which the number of the adjustable variables is the same as the number of the descriptors.

To test the relative contribution of each descriptor, we retrain the rest by leaving one out. The results are listed in Table 3. Without inner-layer-electron descriptors, the RMS deviations increase from 4.4 to 5.5 kcal/mol and from 3.5 to 3.8 kcal/mol for the B3LYP/6-31G(d) and B3LYP/6-311G(2d,d,p) methods, respectively, and for the HF/6-31G(d) method, the RMS deviation increase from 9.5 to 14.7 kcal/mol. In general, inner layer electrons do not contribute much in chemical reactions. Since the calculation of heats of formation is based on an atomization energy scheme, our results

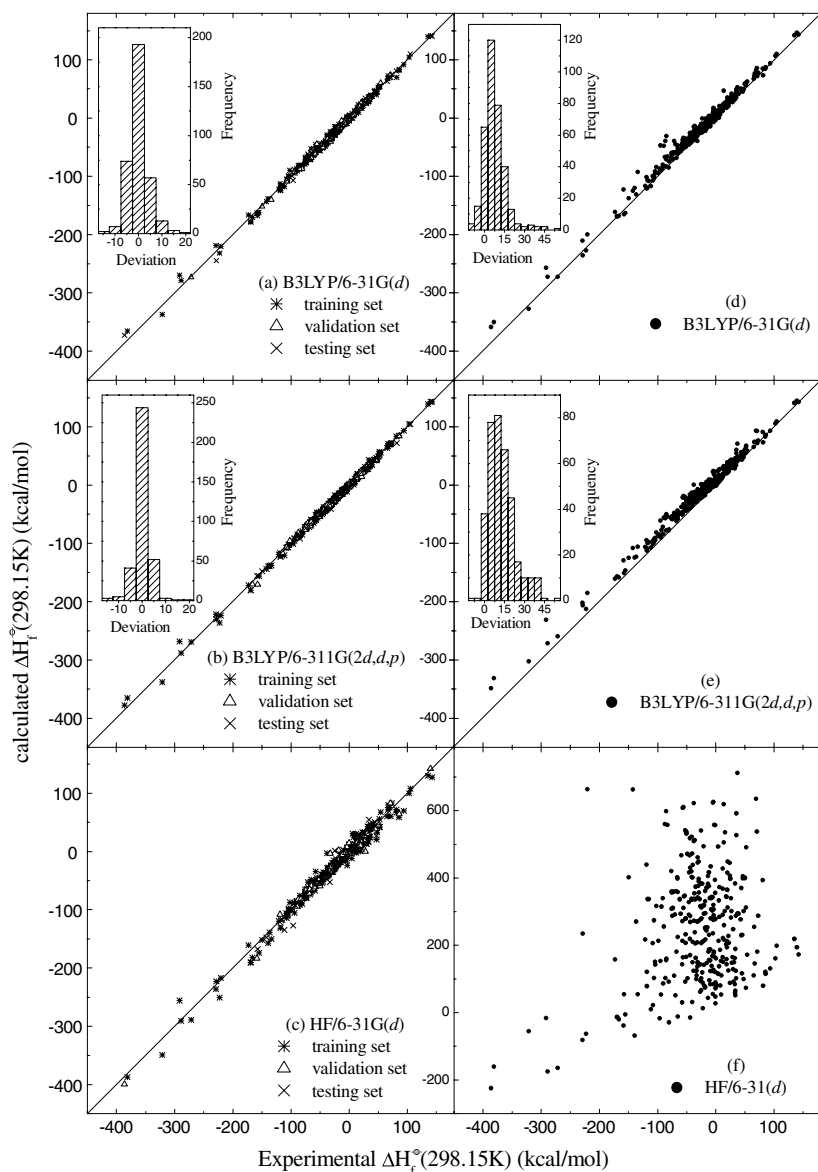


Fig. 2. Experimental versus calculated heats of formation for all 350 molecules: (a–c) neural-network corrected results; (d–f) raw calculated results.

Table 1

The MAD and RMS deviations (kcal/mol) before and after the neural network correction

	B3LYP		HF
	6-31G(d)	6-311G(2d,d,p)	6-31G(d)
B-MAD ^a	8.2	12.4	284.1
A-MAD ^b	3.2	2.3	6.8
B-RMS ^a	11.2	15.2	327.1
A-RMS ^b	4.4	3.5	9.5

^a Before correction.

^b After correction.

surprisingly show that inner layer electrons must be considered in accurately predicting the energy change of a reaction. In addition, when taking the sum of three inner layer electrons as one descriptor, the RMS deviations reach to 5.3, 3.7 and 11.6 kcal/mol for the three meth-

ods, respectively. These indicate that different inner electrons contribute differently to the overall energy change. At the HF level, unpaired electrons of the atoms also have remarkable contributions. Without unpaired-electron descriptor, the RMS deviation increases by 4.6 kcal/mol. In addition, the effect of bonding electrons is slightly larger compared to the effect of lone-pair electrons. Without bonding-electron descriptor, the RMS deviation increases by 0.6 kcal/mol. We consider that the chemical environment is greatly changed upon forming chemical bonds from unpaired electrons in atoms, while the change of chemical environment for the lone-pair electrons from atoms to molecule is smaller. In contrast, for the two DFT methods, the effects of unpaired electrons, bonding electrons, and lone-pair electrons are not so significant. However, without low-occupancy-orbital descriptors (RY*, BD*, LP*), the

Table 2
Weights of the neural network

Weights	B3LYP				HF	
	6-31G(d)		6-311G(2d,d,p)		6-31G(d)	
	y_1	y_2	y_1	y_2	y_1	y_2
BD(a ₁)- Wx_{1j}	-0.5390	-0.1501	-0.6004	-0.7006	0.1467	-0.0100
LP(a ₂)- Wx_{2j}	-0.1371	0.0499	1.8325	-0.0892	0.3760	-0.0061
CR1(a ₃)- Wx_{3j}	-0.7149	0.3169	-0.8559	0.1910	0.2153	0.0194
CR2(a ₄)- Wx_{4j}	-0.6219	-0.4966	0.1429	-0.2580	-0.4025	-0.0277
CR3(a ₅)- Wx_{5j}	0.8161	0.3300	-0.4481	0.1111	0.1792	0.0060
RY*(a ₆)- Wx_{6j}	-0.4773	-0.2331	0.5838	-0.1264	0.2726	0.0030
BD*(a ₇)- Wx_{7j}	0.2355	0.0049	-1.5212	0.0116	-0.2832	0.0172
LP*(a ₈)- Wx_{8j}	-0.2733	0.0399	0.7115	0.1427	0.0223	-0.0015
Unpaired(b ₁)- Wx_{9j}	0.1702	-0.0164	-0.0886	-0.3978	0.4316	-0.1397
Wy_j	0.5420	3.9708	-0.9471	3.5658	-0.3483	-6.9412

RMS deviations of the three methods all increase greatly, which implying that the effects of low-occupancy orbitals cannot be ignored.

In the present work, we have also compared the correction results with different sets of descriptors used in previous work. Firstly, we considered the electron pairs descriptor including the number of bonding electrons, lone-pair electrons, three inner layers electrons, unpaired electrons in molecules, and unpaired electrons in composing atoms in their ground states [20]. There are seven descriptors in that procedure. After the seven-descriptor NN correction, the RMS deviations for the 350 molecules are 5.7, 4.4 and 10.1 kcal/mol for the B3LYP/6-31G(d), B3LYP/6-311G(2d,d,p), and HF/6-31G(d) methods, respectively. Secondly, the original physical descriptors used in Chen's work (the calculated ΔH_f^0 , N_t , ZPE and N_H) were considered as descriptors. The RMS deviations for the 350 molecules reach to 7.9, 5.4 and 19.5 kcal/mol for the B3LYP/6-31G(d), B3LYP/6-311G(2d,d,p), and HF/6-31G(d) methods, respectively. Compared to the results in above two procedures, the RMS deviations (4.4, 3.5 and 9.5 kcal/mol) in this work using NBO descriptors are all decreased for

these three methods, and especially for the HF/6-31G(d) method, the deviations decrease greatly. The reasons may be contributed from number and nature of descriptors used in the neural network procedure. By comparison, it could be suggested that the set of NBO descriptors should be better.

Although the overall results of the neural network correction approach are quite satisfactory, the deviations for the different type molecular systems are still ragged [tabulated in Table 4]. Especially for the non-hydrogen systems, the RMS deviations are significantly larger than the total RMS deviations of the 350 molecules for all the three methods. There are 53 non-hydrogen molecules in the total 350 molecules. The RMS deviations for this type molecules are 7.4, 6.8 and 16.0 kcal/mol for the B3LYP/6-31G(d), B3LYP/6-311G(2d,d,p) and HF/6-31G(d) methods, respectively. For the two DFT methods, the deviations of PF₅, SF₆ and C₂F₆ are above 15 kcal/mol. For the HF method, the deviations for molecules containing fluorine element are especially large, such as for BF₃, ClF₃, F₂O, CF₃Cl, SF₆ and C₂F₆. The large deviations may be attributed to the inaccurate geometries optimized at these levels of theories and other factors unconsidered in the present work, such as spin-orbital coupling and relativistic effects [4,6]. For the inorganic hydrides and radicals, the RMS deviations of the HF/6-31G(d) method are 14.0 and 13.6 kcal/mol, which are still significantly larger than the total RMS deviations (9.5 kcal/mol). In

Table 3
The RMS deviations (kcal/mol) for the neural network with different descriptors

	B3LYP		HF
	6-31G(d)	6-311G(2d,d,p)	6-31G(d)
I ^a	4.4	3.6	10.1
II ^b	4.4	3.7	9.8
III ^c	5.5	3.8	14.7
IV ^d	5.3	3.7	11.6
V ^e	4.4	3.9	14.1
VI ^f	5.7	4.4	10.7
VII ^g	4.4	3.5	9.5

^a Excluding BD descriptor.

^b Excluding LP descriptor.

^c Excluding three-inner-layer-electron descriptor.

^d With three inner layer electrons as one descriptor.

^e Excluding unpaired-electron descriptor.

^f Excluding low-occupancy-orbital descriptor.

^g With all descriptors.

Table 4
Comparison of the RMS deviations (kcal/mol) of different types molecules

	B3LYP		HF
	6-31G(d)	6-311G(2d,d,p)	6-31G(d)
Non-hydrogen (53)	7.4	6.8	16.0
Inorganic hydrides (15)	5.5	3.0	14.0
Radicals (31)	4.1	3.7	13.6
Hydrocarbons (69)	2.3	2.3	4.5
Subst. hydrocarbons (182)	3.7	2.2	6.1
All (350)	4.4	3.5	9.5

contrast, for the two DFT methods, the correction results of the inorganic hydrides and radicals are satisfied for us. For example, for the B3LYP/6-311G(2d,d,p) method, the RMS deviation of the inorganic hydrides even reach to 3.0 kcal/mol. For the hydrocarbons and the substituted hydrocarbons, the correction results are better compared to other types molecules. The RMS deviations of the hydrocarbons are 2.3, 2.3 and 4.5 kcal/mol for the B3LYP/6-31G(d), B3LYP/6-311G(2d,d,p), and HF/6-31G(d) methods, respectively, and for the substituted hydrocarbons they are 3.7, 2.2 and 6.1 kcal/mol, respectively. Compared to our previous LRC method, the corrected results for different type molecules are all slightly better upon the neural network correction. For example, for the B3LYP/6-311G(2d,d,p) method, the RMS deviation of the non-hydrogen molecules is 6.8 kcal/mol upon the NN correction, while upon the LRC correction it is 7.7 kcal/mol [21]. The RMS deviation of the substituted hydrocarbons is 2.2 kcal/mol upon the NN correction, while upon the LRC correction it is 2.7 kcal/mol [23].

5. Conclusion

The neural network correction approach is reemployed to improve the accuracy of DFT and HF calculation with smaller basis set by training the new training set including 350 heats of formation of small and medium-sized organic, inorganic molecules, and radicals. The electron populations of the different types of NBOs are used as new descriptors in present work. They include: 2-center bonds (BD), 1-center core pair (CR), 1-center valence lone pair (LP), 1-center Rydberg (RY*), 2-center anti-bond (BD*), and non-Lewis valence lone pair (LP*). The number of the unpaired electrons of atom in ground state is also included as the descriptor. Upon the NN correction, the RMS deviations for the 350 molecules are reduced from 11.2 to 4.4 and from 15.2 to 3.5 kcal/mol for the B3LYP/6-31G(d) and B3LYP/6-311G(2d,d,p) methods, respectively. At the same time, the calculated ΔH_f^0 s of the HF method have also been improved greatly, and the RMS deviation is reduced from 327.1 to 9.5 kcal/mol for the HF/6-31G(d) method. The NN approach based on the first-principles calculation has been applied to correct other thermo-chemical properties [19] and will be potentially a powerful tool in computational science and in materials research and development.

Acknowledgments

This work was supported by the National Natural Science Foundation of China Grant Nos. (20273015

and 20433020) and the Natural Science Foundation of Shanghai Science & Technology Committee Grant No. (02DJ14023).

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