Full Length Article

A comprehensive exploration of mercury adsorption sites on the carbonaceous surface: A DFT study

Ge Yan[a], Zhengyang Gao[a,*], Mingliang Zhao[a], Weijie Yang[a,*], Xunlei Ding[b]

[a] School of Energy and Power Engineering, North China Electric Power University, Baoding 071003, China
[b] School of Mathematics and Physics, North China Electric Power University, Beijing 102206, China

ABSTRACT

Mercury pollution released from coal-fired power plants has caused worldwide concern for its toxicity, global range transportation, and bioaccumulation. Unburned carbon in fly ash is considered to be a promising adsorbent to effectively remove elemental mercury. However, the active sites of the unburned carbon for Hg^0 adsorption have not been clearly identified, which greatly hinders the development of effective adsorbents. To reveal the adsorption sites of the carbonaceous surface, the adsorption process of Hg^0 on different carbonaceous surfaces was systematically investigated through density functional theory. The Mayer bond order, Electron localization function, and Electron density difference were used to analyze the adsorption mechanism of Hg^0. Meanwhile, the oxygen-containing functional groups were also considered to research the influence on mercury adsorption with the defective surface. The adsorption of Hg^0 on defective carbonaceous surfaces is associated with stable chemisorption, and surface defects can significantly improve the adsorption energy of Hg^0. This theoretical study provides theoretical guidance for the development of mercury removal technology with carbon materials in the coal-fired power plant.

1. Introduction

Currently, mercury emissions have been a global concern due to its toxicity, stability to be transported in the environment, affecting the nervous system and can cause severe disability [1-3]. The coal-fired power plant is universally considered to be the largest source of mercury emissions. Therefore, solving the problem of mercury emissions from coal-fired power plants has become the main aspect of global mercury emission control [4,5]. It is a consensus that elemental mercury (Hg^0), oxidized mercury (Hg^{2+}), and particulate-bound mercury (Hg_p) are three forms of mercury emissions in the flue gas of coal-fired power plant [6]. Mercury oxide is soluble in water, so it can be removed with high efficiency by wet flue gas desulfurization (FGD) equipment [7]. Besides, most particulate mercury can be removed by air pollution control devices (electrostatic precipitators (ESPs) or fabric filters). On the contrary, because elemental mercury is insoluble in water and has higher volatility, it is difficult to capture by dust removal equipment or desulfurization equipment [8-11]. Hence, among the three species of mercury found in coal-derived flue gas, how to effectively remove the elemental mercury from flue gas is a hot topic for researchers.

At present, the oxidation and adsorption are two main technologies to control mercury emissions. For the oxidation, it was reported that selective catalytic reduction (SCR) device not only can reduce NOx to nitrogen but also promote oxidation of Hg^0 effectively [12,13]. The pilot test of EERC (Energy and Environmental Research Center) also reported that after burning high chlorine bituminous coal through SCR, the particulate mercury has a significant increase while burning low chlorine bituminous coal has no significant change [14]. Besides, through analysis of the reactivity, selectivity, and mechanism of different radicals in mercury removal, the chlorine-containing radicals can effectively oxidize Hg to Hg^{2+} [15,16]. Finally, V_2O_5 [17,18] and MnO_2 [8,19,20] have the catalytic oxidation effect of Hg^0 to Hg^{2+}. For the adsorption, the mercury capture rate can be higher than 60% by adding activated carbon injection technology at the entrance of electrostatic precipitator (ESP) equipment, and it can be increased to 90% by using filter type precipitator [21]. Additionally, both the CaO [22,23] and Fe_2O_3 [24-26] also have a positive effect on removing mercury from flue gas. However, these catalysts or technologies have the disadvantages of high cost, poor thermodynamic stability, and lower removal efficiency. In recent years, carbon surface catalysts have become a popular topic.

Fly ash is an industrial by-product produced in the process of coal-fired power generation [27-29]. It can be used as a low-cost adsorbent to absorb various harmful substances such as VOCs (volatile organic

compounds) [30,31]. The idea of using recycling fly ash for metals was first proposed by Owens et al. [32]. The fly ash would be injected into the flue gas train control device, similar to the use of activated carbon, thus saving a lot of capital and adsorbent cost. Serre et al. [33] explored the adsorption of mercury on fly ash by experiment. The result showed that the fly ash with carbon content between 2% and 35% has a large amount of Hg^0 adsorption and when the adsorption reaches equilibrium, the concentration of Hg in the adsorption phase is directly proportional to the carbon content in the fly ash. With the increase of carbon content, the Hg of the adsorption phase increases. Besides, fly ash has excellent adsorption performance for lead [34], heavy metal atoms in water [35-37], and organic pollutants [38,39]. These experimental studies show that fly ash has very good properties for adsorption of harmful substances. But in the actual reaction process, the reaction between them is very complex and many thermodynamic and kinetic data cannot be obtained directly. Obviously, the theoretical calculation can solve this problem and show the characteristics that the experiment cannot show. Recently, a large number of scholars have studied the adsorption mechanism of elemental mercury on the carbon surface by theoretical calculation. This will help to find more economical and effective ways to control mercury emissions.

The benzene cluster is often used as the model to simulate the carbonaceous surface such as graphene, active carbon, and unburned carbon in fly ash when researching the adsorption mechanism between the mercury and carbonaceous surface. In the theoretical study, the adsorption mechanism of mercury by the zigzag and armchair model was proposed for the first time in 2011 [40]. The result showed that active states can directly absorb the element mercury and the halogen atom can improve the ability to capture elemental mercury. Then modified by various chemical functional groups, such as sulfur dioxide [41], sulfur trioxide [42], and the oxygen functional groups [40] have been reported to investigate the effect on mercury capture capacity of the carbonaceous surface. Among these chemical substances, researchers have different views on the role of oxygen functional groups in capturing elemental mercury on the carbonaceous surface. The experimental research results on X-ray absorption fine structure (XAFS) spectroscopy indicate that the oxygen atom may provide the active site for Hg^0 bonding [43]. Some studies have shown that oxygen functional groups have inhibitory effects on the adsorption with mercury [44,45], but other studies have shown that they have promoting effects [46-48]. Recently, the single-atom catalyst with graphene-based substrates is widely used in various catalytic fields and it was reported that Fe/SV-N3 has a strong ability to capture elemental mercury [49]. Through the introduction of the above research, we found that no matter in the theoretical calculation or the experiment, scholars ignored the real sites on the adsorption performance of the carbonaceous surface. He et al. [50] only discussed one kind of defective carbonaceous structure to research the active site with mercury adsorption which is a lack of unified and systematic research. In fact, many defective structures occur in the carbon particles and unburned carbon in fly ash [50-52]. Therefore, it is very helpful for us to study the adsorption sites of mercury on the carbonaceous surface. To supplement and develop the adsorption sites of mercury capture by unburned carbon in fly ash. We have studied the process of mercury adsorption by defective structure and it is the first time to simulate various carbonaceous defective structures to explore the active sites of mercury adsorption. Meanwhile, consider the various oxygenated functional groups in the carbonaceous surface, we also researched the influence of oxygen-containing functional groups on adsorption of elemental mercury by the defective carbonaceous structure.

In the present study, the density functional theory (DFT) calculation on the adsorption mechanism of elemental mercury on the defective carbonaceous surface is proposed. Firstly, the twelve kinds of defective carbonaceous surfaces were simulated and the strength of the active site was evaluated by Atomic Dipole Moment Corrected Hirshfeld (ADCH) charge [53]. Secondly, all of the possible structures of mercury

adsorbed on the edge sites of the defective carbonaceous surface are considered to examine their effects on Hg^0 adsorption. Then the Mayer bond order (MBO), electronic localization function (ELF), and electronic density difference diagram were utilized in three configurations with the largest adsorption energies to analyzing the interaction between elemental mercury and defective carbonaceous surface. Finally, the effect of oxygen functional groups (semiquinone, lactone phenol, and carbonyl) with mercury adsorption on the defective carbonaceous surface was analyzed. This work can fully reveal the real active sites on the adsorption of mercury on the carbon surface, and also reveal the effect of oxygen functional groups on the adsorption of mercury on the defective carbonaceous surface.

2. Calculation method

In this work, the quantum chemistry method was applied to simulate the adsorption process of mercury on the defective carbonaceous surface. The structures of all the adsorption models were calculated by the geometric optimization and frequency calculation. Considering the effect of spin multiplicity, we choose the structure with the lowest energy as the ground state structure from three kinds of spins.

Density functional theory (DFT) was applied to calculate structural properties because it provides a good balance between calculation efficiency and accuracy. Among them, the B3LYP algorithm, one of the most popular methods, has been used in many kinds of literature because it can produce fairly thermodynamic properties of reactions and accurate bond energies [54-56]. Besides, the def2-SVP [57] basis set also be used to improve the accuracy and reliability of calculation. Therefore, this theoretical level is a reasonable plan, which can be completed within the acceptable calculation cost. The specific calculation details are: during all the geometry optimization, the def2-SVP basis set was utilized to C, H, O and Hg atoms, the single point energy was calculated by the def2-TZVP basis set. The virtual frequency was checked by frequency analysis to confirm the stability of the structure, meanwhile, zero-point energy and thermodynamic data were obtained. The DFT-D3 was applied to correct the weak interaction force under the condition of fully considering the weak interaction force to improve the calculation accuracy. Finally, the Gaussian 09 software package was used for all above the calculations [58].

The adsorption energy (E_{ads}) is a crucial standard of criterion to reveal the mechanism of the adsorption process. The adsorption process of molecule A on solid surface B is exothermic. The calculation formula of system energy is as follows:

$$E_{ads} = E_{AB} - (E_A + E_B)$$

where the E_{ads} is the adsorption energy, E_{AB} corresponds to the total energy when molecule A adsorbed on the solid surface B, E_A and E_B are the total energy of molecule A and solid adsorbent B in the ground state. As we all know, the adsorption energy has two types. One is the physical adsorption process which corresponding to less than -50 kJ/mol. The other is that the adsorption energy is more than -50 kJ/mol which belongs to the chemical adsorption process.

3. Results and discussion

3.1. Research model

Recently, the single graphite layer is often used to simulate the carbonaceous surface and it is proved to be highly consistent with the experimental results. Chen et al. [59] have researched the molecular orbital of six kinds of graphene monolayers with increasing the number of benzene rings using the quantum chemistry method and the conclusion claimed the calculated results are in good agreement with the experimental data. Montoya et al. [60] found the activity of the carbonaceous model did not depend on the size and the edge shape. Therefore, to obtain a stable defective structure with three defects,
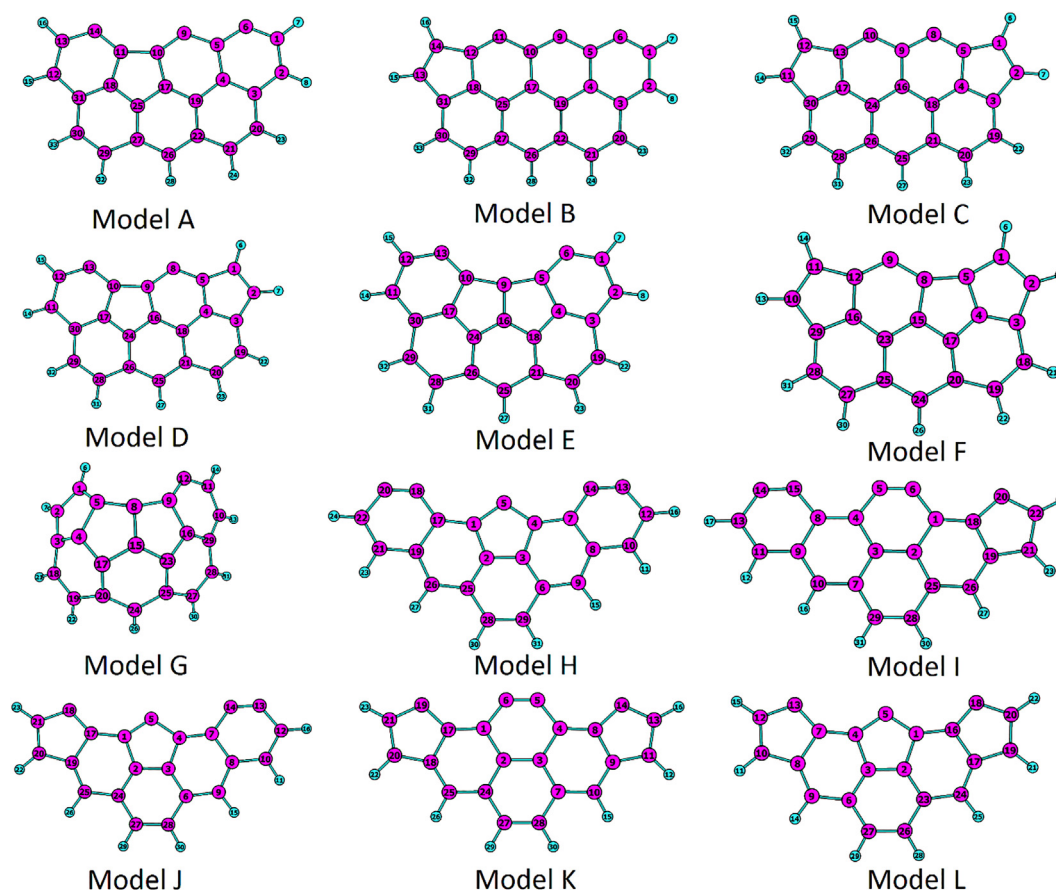
Fig. 1. Models of the defective carbonaceous surface (violet: C turquoise: H). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

seven benzene rings were selected to simulate the carbonaceous surface in all the calculations. The edge atoms on the upper side of the models are bare to simulate the active sites and the other edge atoms are besieged by saturated hydrogen atoms. Although in the actual reaction, there is no saturated hydrogen atom or other hybrid atoms on the edge of graphene, considering the suitable adsorption environment and charge balance, using saturated hydrogen atom is still a feasible method. Besides, single edge carbon atoms are enough for many applications and it's very consistent with our previous work [55,61].

The defective carbonaceous surface evolved from the non-defective carbonaceous model, it contains three kinds of structures that represent single, double, triple defects respectively. The optimized defective carbonaceous surface by DFT calculation is illustrated in Fig. 1. The carbon atoms and hydrogen atoms are labeled with different numbers to distinguish them in later discussions. Model A to G is formed by the evolution of the zigzag edges and the model H to L is formed from the armchair edges. There is a phenomenon that is different from the defective zigzag model: the absence of carbon atoms does not form vacancies but form many five-membered rings in the defective armchair model. The dihedral angles of optimized models are either 0° or 180° suggesting that these models are consistent with previous studies [55,61], but the model G is 122.92°, indicating that the structure of carbon surface will bend to a certain extent to achieve steady state. Besides the result data, including bond lengths and bond angles are consistent with the previous research [62].

3.2. ADCH charge on defective carbonaceous surface

The ADCH charge analysis is applied to calculate the charge distribution in the models, which cannot be measured in the site. It has

been extensively used in the studies of atomic charge distribution and transfer in molecules because of its good physical significance and low selectivity for base groups and functional. Additionally, it also has the advantages of short calculation time, high accuracy, and so on. The computational result of models are listed in Table 1 and Table 2, which corresponding to the defective zigzag edges and armchair edges. The Table 1 listed ADCH charge data of seven models which corresponding to model A to model G. It can be seen that C6, C9, C14 of the model A have more negative charge indicating that these active sites are more likely to attract free radical electrons. When there are defects caused by losing two carbon atoms on the carbonaceous surface, the number of negative charges are: C8 and C10 are zero in the model C; C8 and C13 are −0.03 and −0.01 in the model D; C6 and C13 are −0.01 in the model E respectively. Compare to the three models, model D seems like have more strong ability to adsorb the other element. Then the active site (C12) of the model G has the lowest negative charge (-0.08) in the seven carbonaceous surface models.

Table 1
The ADCH charge of defective carbonaceous surface with zigzag edges.

	Model A	Model B	Model C	Model D	Model E	Model F	Model G
C5	0.00	−0.02	−0.03	0.00	0.00	0.02	0.00
C6	−0.01	−0.01			−0.01		
C8			0.00	−0.03		0.00	0.00
C9	−0.05	0.01	−0.01	0.00	0.06	−0.01	0.00
C10	0.02	−0.02	0.00	−0.02	0.00		
C11	0.01	0.01					
C12		−0.02				−0.03	−0.08
C13			−0.03	−0.01	−0.01		
C14	−0.03						

Table 2
The ADCH charge of defective carbonaceous surface with armchair edges.

	Model H	Model I	Model J	Model K	Model L
5C	0.03	−0.04	0.00	−0.04	0.00
6C		−0.03		−0.04	
13C	−0.04		−0.04		0.00
14C	−0.04	−0.04	−0.04	0.01	
15C		−0.04			
18C	−0.04		−0.01		0.00
19C				0.01	
20C	−0.04	0.02			

In Table 2 there's a very different result and it reveals a phenomenon that no one has ever noticed. It is that when the armchair model appears five-membered ring which also caused by losing the carbon atoms, the active sites in the five-membered ring carry the positive charge or as a neutral atom. The active sites in each defective model have a positive or zero charge and the positive charge is relatively large in model H and model I. The zero charge sites appear from model J until all the active sites become neutral atoms in model L. From the above calculation results, we can conclude that the activity of zigzag defective models is greater than that of armchair defective models. Although the electronegativity of armchair defective models is larger than that of zigzag defective models, there are also sites with a positive charge, which have a great influence on these models, so the activity of armchair defective models is lower than that of zigzag defective models.

3.3. The adsorption with Hg^0 on the defective carbonaceous surfaces

The optimized geometries of all the above models interact with Hg^0 are calculated respectively and all the configurations have converged. The optimized models with mercury adsorption are shown in Fig. 2 and the adsorption energies with mercury are listed in Fig. 3. To distinguish it from the label of the adsorbent model, Model (a&b) is applied to represent the adsorption system. It can be seen from the Fig. 2 and Fig. 3, in the first category of defect, compare to the model B(a&b) and model I(a&b), model A(a&b) and model H(a&b) have higher adsorption energy, which corresponding to −212.79 kJ/mol and-62.73 kJ/mol it reveals that the model with defects in the middle position is better than that in the position of both ends. And the model A(a&b) also proved to be the best structure for the adsorption with mercury on defective carbonaceous surface. For the second category of defects, they contains five models: model C(a&b), model D(a&b), model E(a&b), model J(a&b) and model K(a&b). Except the model K(a&b), the adsorption energies of four models are more than −50 kJ/mol which belong to the chemical adsorption. Among the five models, the zigzag defective carbonaceous surfaces are better than the armchair defective carbonaceous surfaces which is consistent with the calculation result of the ADCH charge. In addition, the adsorption energy of mercury adsorption on model E(a&b) (-183.55 kJ/mol) is higher than model C(a&b) (-54.72 kJ/mol) and model D(a&b) (-64.14 kJ/mol), which means that the surface with two continuous defects is better than that with discontinuity. And it also be proved by the adsorption energy between model J(a&b) (-77.76 kJ/mol) and model K(a&b) (-43.30 kJ/mol). For the calculation result of the ADCH charge, the reason why the adsorption energy of model E(a&b) is greater than that of model D(a&b) is explained in the supplementary material. When discussing the surface which contains triple defects, there are three models: model F(a&b), model G(a&b), and model L(a&b). The adsorption energy with mercury adsorption on model G(a&b) (−118.50 kJ/mol) and model L(a&b) (-81.60 kJ/mol) is higher than model F(a&b) (−59.02 kJ/mol) which is also consistent with the above conclusions.

To quantitatively analyze the difference of adsorption energies between all configurations, the Mayer bond order is carried out to analyze C–C and C-Hg bond. It has been used in many fields of quantitative

calculation since it has strong universality (organic, inorganic, and transition metal bonding can be used) and easy-understanding characteristics. Additionally, it can also well reflect the physical and chemical nature. Some optimized bond lengths and Mayer bond order are listed in Table. S3 and Table. S4 (in the Supplementary Material). Firstly, it can be seen from the results, when the carbon surface is defective, the MBO and bond length of C–C have a great change in the zigzag model but not in the armchair model. These results reveal that the influence of defects in the zigzag model is greater than that in the armchair model. Secondly, the bond length of C-Hg on model A(a&b), model D(a&b), and model E(a&b) have smaller bond length and MBO values are greater than 0.7 which indicated that the strong interaction between mercury and these surfaces is established. For the armchair model, the bond length of C-Hg is similar to that in the zigzag edge and the MBO value also can reach 0.7(model J(a&b) and model L(a&b)). However, due to the electron distribution at the edge of the armchair, even if it has the similar data to the zigzag edge, it cannot get a quite high adsorption energy.

3.4. Electron localization function analysis

Mayer bond order grade quantitatively analyzes the bonding strength and the number of shared electron pairs between the element mercury and the defective carbon surface. Electron localization function (ELF) is a super important real space function to study the electronic structure of a chemical system. It can show the electronic localization degree of different positions in three-dimensional real space, and it is easy to calculate and analyze figures. It is an important tool in the field of quantum chemistry to study the characteristics of electronic structure. ELF analysis will more intuitively understand the strength of the interaction between the element mercury and the defective carbonaceous surface from the graph. In Fig. 4, we only discussed three adsorption configurations with the largest adsorption energy and the complete zigzag model with mercury adsorption to analyze the bonding between mercury and carbonaceous surface. In Fig. 4 (a), C–C is connected by a stable covalent bond and the surrounding hydrogen atoms are surrounded by lone pair electrons in this section. In the zigzag (a&b), there are still free lone pair electrons around the mercury atom. The electrons between the C-Hg bond are concentrated around the carbon atom, and the contact area of the two-electron cloud is small. This phenomenon also verified the reason for low adsorption energy with mercury on the non-defective carbonaceous surface. In model A (a&b) and model E (a&b), the electron cloud of mercury atom is completely fell into the vacancy generated by the defect, which reveals that the vacancy has a stronger ability to absorption with mercury. Compare to model E (a&b), model A (a&b) has higher electronic localization between C-Hg bonds which is consistent with the adsorption energy. To explain the difference of adsorption energy on Zigzag (a&b) and model G (a&b), electron density differences of the reactions were calculated and the results are shown in Fig. 4 (b). In the graph, dashed lines and solid lines correspond to the regions where the electron density is decreased and increased respectively. It can be seen that there are isolated electron clouds around the mercury atom in Zigzag(a&b) and model G (a&b) but the difference is no overlap of electron cloud between the C-Hg bond in Zigzag (a&b). Such a result which is not reflected in the ELF diagram directly shows the reason for the difference of adsorption energy between the two models, and also demonstrates the reason for the low adsorption energy of Hg^0 on complete zigzag model with the field of electronic density.

3.5. Effect of oxygen functional groups on Hg^0 adsorption on defective carbonaceous surface

In recent years, many researchers have reported that the carbonaceous surface contains many different types of oxygen functional groups and the carbon–oxygen complexes are the most important
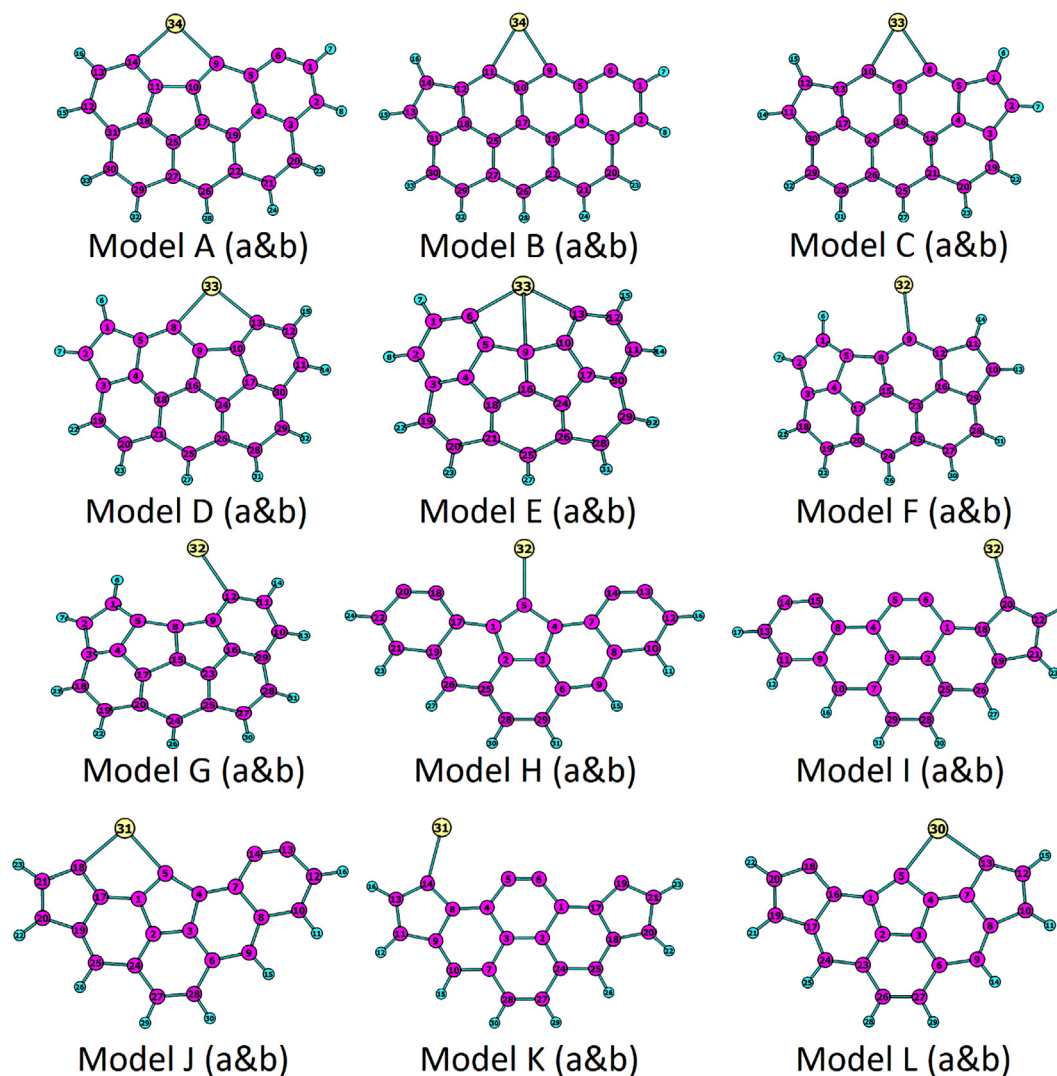
Fig. 2. The optimized models with mercury adsorption on defective carbonaceous surface (violet: C turquoise: H yellow: Hg). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

structures which influence the surface characteristics and adsorption properties of the carbonaceous surface [44,47,55]. Depending on the number of oxygen and hydrogen, they could be phenolic, lactone, carboxyl, and carbonyl groups. For the adsorption with mercury, there are reported that different oxygen functional groups have different effects [40]. For lactone, carbonyl and semiquinone functional groups, they can enhance the ability of adsorption of mercury while the phenol and carboxyl groups show a physisorption with mercury[40,44]. Since these three kinds of surfaces (model A, model E, and model G) have the largest adsorption energy for Hg^0 and they are the most typical defective surface with certain representativeness. Therefore, these kinds of defective carbonaceous surfaces modified by four oxygen functional groups were investigated for the influence on mercury adsorption to see if they reach the same conclusion. The optimized structures with mercury adsorption on defective carbonaceous surfaces modified by oxygen functional groups are illustrated in Fig. 5, C-Hg bond lengths and adsorption energies are listed in Fig. 6.

From the results of calculation, we got almost the same conclusion that the Hg^0 atom tends to adsorb with the carbon atom. But there are some new discoveries which are the Hg^0 atom interacting with the oxygen atom on model A and model E which are modified by the semiquinone functional group. Through the analysis of Hg^0 adsorption energy, it was found that the lactone, phenol, carbonyl, and model G modified by the semiquinone don't improve the ability of adsorption

with mercury which is inconsistent with the previous results [40,44]. Only the semiquinone on model A and model G favor the chemisorption of mercury since it interacts with the oxygen atom. The bond length of Hg-O is 2.27 Å and 2.14 Å which are less than 3 Å, indicating that the Hg^0 atom may have oxidation with the oxygen atom and it demonstrates the research findings on X-ray absorption fine structure (XAFS) spectroscopy [63]. From the above discussion, we know that compare with the previous results, there are some different conclusions with the adsorption of Hg^0 on the defective carbonaceous surface modified by the oxygen functional group. In the current calculation result, compared with the complete carbon surface with oxygen functional groups, the semiquinone on the model A and model E promote mercury adsorption while the lactone, phenol, carbonyl groups may inhibit the adsorption with Hg^0 and the inhibition is most severe on the model G. Therefore this result gives us a revelation that we should not only consider the influence of the types of oxygen functional groups on mercury adsorption but also consider the influence of the defects on the carbonaceous surface.

From all above the discussion, all possible defective structures on the carbonaceous surface were established to research the influence of adsorption with elemental mercury. Through the ADCH charge analysis, we can conclude that the carbon atoms with zigzag edges are more active than those with armchair edges. Among all the models, the model A is considered to the best structure to absorb the elemental
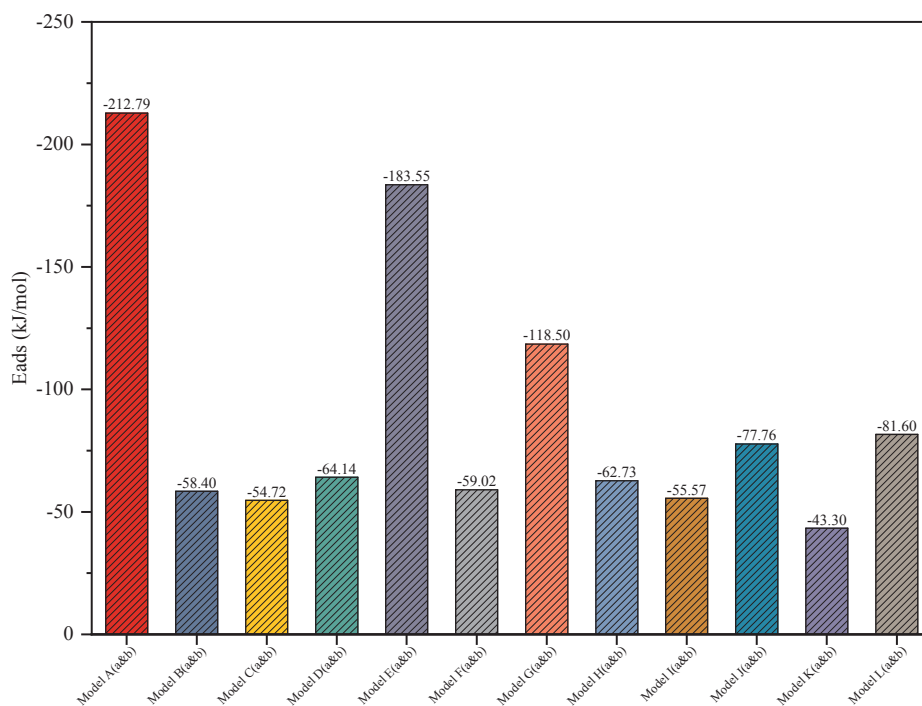
Fig. 3. The adsorption energy with mercury adsorption on defective carbonaceous surface.

mercury and it was proved by calculation of adsorption energy. Additionally, the adsorption energies of other adsorption structures are also within the scope of chemical adsorption, except for model K(a&b). Then electron localization function and electron density differences explained the reason for chemical adsorption with mercury when it reacts with these surfaces in the field of electronic density. And the conclusion is that there is an overlap of electron cloud between mercury and surface, and the degree of overlap determines the adsorption capacity. Finally, to make the model closer to the real carbonaceous surface, the influence of oxygen-containing functional groups on the adsorption of elemental mercury is also considered. The calculated structure shows that only model A and model E modified by Semiquinone improve the adsorption capacity of mercury while other

oxygen functional groups have no obvious promotion effect.

4. Conclusion

In this work, the adsorption sites of Hg^0 were investigated systematically adopting defective carbonaceous surfaces with zigzag and armchair edges in the computing way of density functional theory. This research may help to open up another dimension for the mercury removal from the coal-fired power plant. After performing model analysis, calculation of adsorption energy, bond level analysis, ELF and electron density difference discussion and the influence of oxygen functional group, we gain the following results:
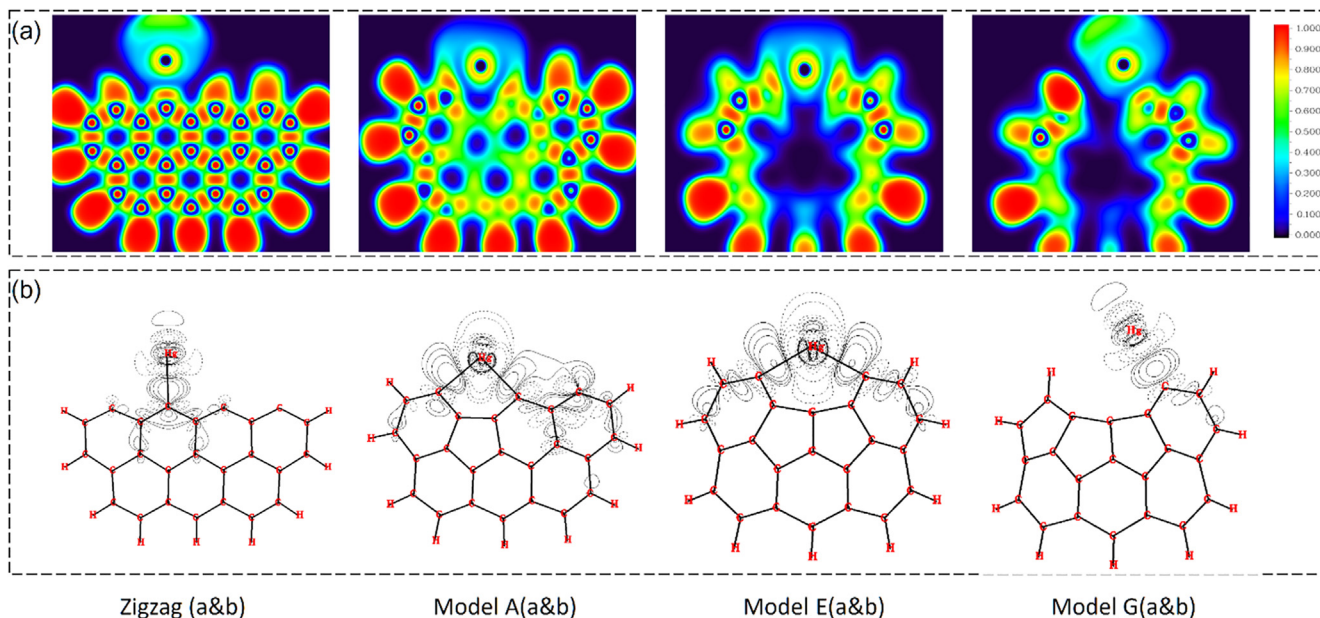

Fig. 4. (a) Electron localization function (ELF) distribution maps, (b) Electron density differences diagram.
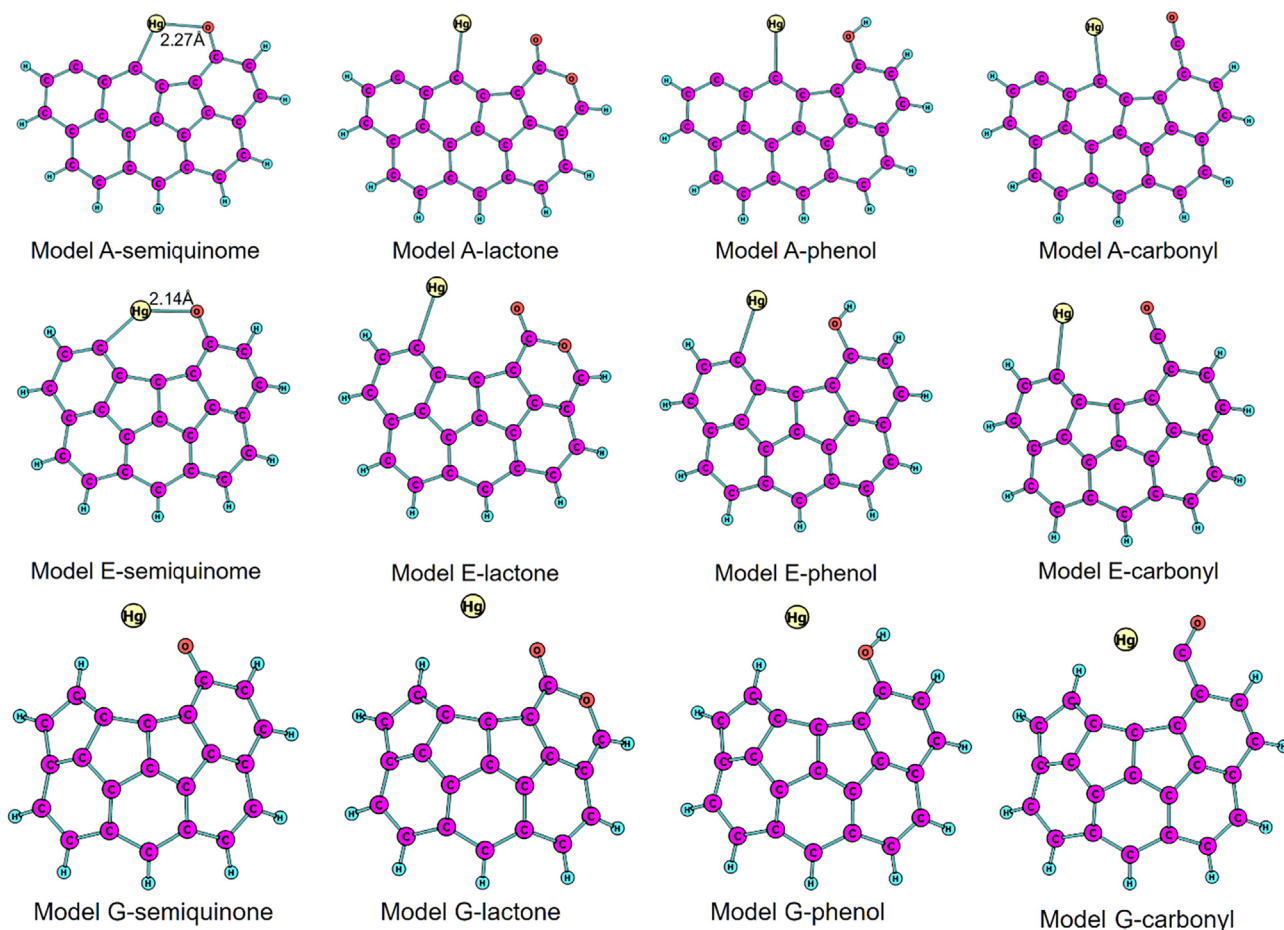
Fig. 5. Adsorption of Hg^0 on defective carbonaceous surface with oxygen functional groups.
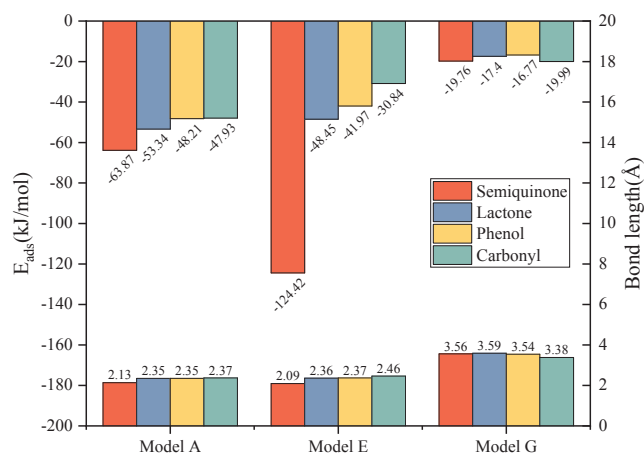

Fig. 6. The bond length of C-Hg and adsorption energies with Hg^0 adsorption on defective carbonaceous surface with different oxygen functional groups.

1) The chemical properties of defective carbonaceous surface no matter zigzag edges or armchair edges are better than the non-defective carbonaceous surface which is quite important for the adsorption with harmful substances.

2) Compare with the complete surface, the reaction of Hg^0 with the defective surface releases more heat (-44.6 kJ/mol for zigzag and −48 kJ/mol for armchair [40]). The adsorption energies of model A(a&b) to model J(a&b) and model K(a&b) are higher than −50 kJ/mol which is indicated that they all within the scope of chemical adsorption while a physical adsorption between the Hg^0 and model

K.

3) With the electron localization function and electron density differences, it can be found that vacancy is the real adsorption site of mercury chemisorption on carbonaceous surface.

4) For the effects of oxygen functional groups, the conclusion is: only semiquinone favors the chemisorption of Hg^0 because the oxygen atom also as the active site to interact with the Hg^0 while the other groups show physisorption of Hg^0.

Conflict of interest

To the best of our knowledge, the named authors have no conflict of interest, financial or otherwise. All authors have completed the disclosure form in the guide for authors and declare that: (1) no support, financial or otherwise, has been received from any organization that may have an interest in the submitted work, (2) there are no other relationships or activities that could appear to have influenced the submitted work.

CRediT authorship contribution statement

Ge Yan: Data curation, Visualization. **Zhengyang Gao:** Software, Supervision, Funding acquisition, Resources. **Mingliang Zhao:** Investigation, Conceptualization. **Weijie Yang:** Methodology, Funding acquisition. **Xunlei Ding:** Writing - review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial

interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.fuel.2020.118781.

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