Synergetic effect of N/P/B coordinated Fe/Co on carbon support catalysts for removing odor-chemicals of cooking source

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Abstract

Odor-chemicals from cooking source have cancer risk for family members and commercial kitchen workers. They are now enabling O₃ formation and beginning to enter the one of the main pollutants in life. The diffusion of odor-chemicals is due to scarce adsorbing materials in range hoods, resulting in urgency of design and development of low-cost materials. Catalytic methods involving oxidation and incineration of odor-chemicals have been explored. Following basic research for catalysts have been focused on catalytic performance, process, activity sites, stability and storage capability. Herein, we calculated reaction process between Fe/Co–N/P/B–C catalysts and CH₄ using density functional theory method. The catalytic performance of nitrogen and phosphorus or boron dual-coordinated iron or cobalt atoms on carbon material was discussed. Total activation energy required for these catalysts was decreased relative to Pt/C. Based on the results of charge density and projected density-of-states, we found that strong Fe/Co 3d electron composition and electron transfer from N 2p/P 3p to Fe/Co 3d were highly dispersed on carbon material, activity sites formed at the surface of materials could efficiently migrate and storage CH₄ and enhance the catalytic capability and stability. The work presented herein highlights the importance of density functional theory method quantified synergetic effects on material properties and more importantly demonstrated the potential of active sites toward enhancing the storage capability and stability of materials for practical applications.

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Graphic abstract

Keywords Odor-chemicals · Density functional theory · Non-noble catalyst · Activity sites · Storage capability · Stability

1 Introduction

The Chinese style dishes are well-known and have been widely selected in daily life [1, 2]. There are odors and fumes spreading at indoor and outdoor air during cooking activities. However, range hoods in kitchens have limit of removing odors [3, 4], particularly when oil-based cooking methods are the primary process [5]. Thus, main odor-chemicals, for instant, carbonyls (C1–C8) are needed to be environment-friendly removed so that minimum effect in term of human health and outdoor air within the specific

range [3, 6]. In the odor-chemicals of cooking source, volatile aldehydes have certain effects in inducing lung cancer and respiratory illness [7–9], moreover, these odor-chemicals are active at occurring volatile chain-scission reactions to form methane [10], consuming NO_x (nitrogen oxide) in air to form O₃ under high temperatures, electrostatic precipitators, strong light and oxidizer [11–13].

In recent years, increasing basic research for catalyst is the result of a concerted effort on concerning odor-chemicals leading to decreased odor exhaust from range hood [14–20]. Discovery of single-atom catalysts along with an

in-depth understanding for their activity, storage capacity and stability have played a major role in developing control technology. It has been suggested that honeycomb carbon supported Pt catalyst are characterized with high activity under moderate-temperature, thus leading to incineration of cooking oil fumes [20]. Meanwhile, single atom silver supported over Mn_2O_3 has been exhibited high activity, storage capacity and stability, thus facilitating the oxidation process of hexanal [17]. However, noble metals (Pt and Ag) have limit of wide application due to high cost.

Recent studies indicated that catalytic activities of single-atom catalysts (SACs) with non-noble metal were also related to carbon material constitution, such as high catalytic performance can occur in Fe–N–C electrocatalyst with dense active sites because of enhanced external surface area and mesoporosity [21–24]. Indeed, in low-cost fabrication of Fe–N–C catalyst made through surface dangling bonds showed maximum atom economy and superior performance for various catalysis fields [25]. In addition, it has been reported that Co–N–C catalyst shows similar structure with Fe–N–C catalyst [26], consequently, Co–N–C catalyst also can be explored, particularly with respect to removing odor. Otherwise, synergistic Fe–N–C–B and Fe–N/P–C species had boosting effects for electrocatalysts and outperformed the Pt/C benchmark [27–29]. Thus, nitrogen and phosphorus or boron dual-coordinated iron or cobalt atoms on carbon material are available to catalyze odor [30]. Therefore, the quest for catalytic mechanism necessitates detailed investigation of charge transfer and activation energy of catalytic process that indicates performance of catalyst. In terms of catalytic mechanism, recent

reports on single-atom catalysts have suggested that the use of Al-doped graphene (refs [31].) and M/g- C_3N_4 (M=Fe, Co, Ni; ref [32].) structure can facilitate acetaldehyde adsorption and detection as well as CO_2 reduction, respectively, which benefits from the effects between chemicals and the activity sites.

In a similar vein, we report a thorough study of Co/Fe–N/P/B–C catalysis carbonizing representative odor-chemicals of cooking source, namely, methane. We analyze: (1) energy consumed due to microstructural changes; (2) activity sites according to electron property; (3) storage capacity and stability based on diffusion path. Catalyst structure used allowed us to obtain reference parameters of graphene from Materials Project (MP) database [33]. This article will serve as an embodiment of how calculation with density functional theory method can work to light possibility in science and technology, conducting researchers to make commercial catalysts.

2 Computational methods

First-Principles Calculation A classical and efficient Vienna ab initio simulation package (VASP) with the periodical density functional theory (DFT) methods was used [30, 34, 35], incorporating generalized gradient approximation (GGA) using the Perdew–Burke–Ernzerhof (PBE) exchange–correlation functional [36]. The plane-wave cutoff energy of 400 eV was employed. A vacuum distance of ~ 15 Å was used on (001) surface of Fe/Co–N/P/B–C to avoid interaction between adjacent layers.

Fig. 1 Projected density-of-States for catalyst: **a** Fe–N–C; **b** Co–N–C; **c** Fe–N₃P–C; **d** Pt–C

Fig. 2 Charge density for catalyst surface (001): **a** Fe–N–C; **b** Co–N–C; **c** Fe–N₃P–C; **d** Pt–C

Climbing-Image Nudged Elastic Band Calculations To investigate the odor storage capacity on catalyst surface, the odor (e.g., CH₄) migration mechanism was determined using the climbing image nudged elastic band (CI-NEB) method based on DFT-calculated energies [37]. The migration paths were considered by CH₄ diffusion on the catalyst (001) surface.

3 Results and discussion

3.1 Electron property

To further investigate active sites of these single-atom catalysts, projected density of states (PDOS) was calculated. As shown in the PDOS (Fig. 1a, d and Fig. S2), the presence of strong Fe/Co 3d component below and near the Fermi level indicates the stability of 3d electrons around Fe/Co atoms. Moreover, there are pronounced overlap between Fe/Co 3d and N 2p/P 3p orbitals above the Fermi level, indicating that charge transfer from N 2p/P 3p to Fe/Co 3d. Their activity sites mainly originate from electrons of N 2p/P 3p contributed to Fe/Co 3d orbital. This is further supported by the formation of core electrons around Fe/Co atoms, as shown in the charge density analysis (Fig. 2). Compared with the PDOS characteristics of these

single-atom catalysts, the Pt atom with weak 5d component below and near the Fermi level and there is not overlap between Pt 5d and C 2p orbitals above the Fermi level (Fig. 1d), indicating that the covalent bonds and core electrons in platinum atom attribute to stability and catalysis, being consistent with charge density analysis (Fig. 2).

Accessing nitrogen or phosphorus atom in carbon material resulted in destabilization of core electrons on (Fe and Co) atoms (charge density greater than 0.5) (Fig. 2a–c). Among, a coordinate bond (Fe ← N–C) and strong Fe 3d electron composition in Fe–N–C system enhance charge density around iron and nitrogen atoms (Fig. 2a). There is an empty 3d orbital for cobalt coordinated with nitrogen and carbon atoms, thus the high charge density around cobalt and nitrogen atom as seen in Fig. 2b. There are similar classes of catalysts, involving optional P: 3p³ and B: 2p¹, effects to replace nitrogen have to start with an understanding of what makes the nitrogen so outstanding within catalyst composition. Originally, nitrogen atoms are introduced into carbon materials itself. Although carbon material has high cycling stability because of lattice stability, it also has weak active sites. For these reasons, carbon atoms are replaced with nitrogen atoms as active sites. Because phosphorus atom has bigger radius than nitrogen and charge density on phosphorus atom are lower values than on nitrogen atoms (e.g., Fig. 2c). Instead there is

Fig. 3 Removing process of CH₄ on Fe–N–C (001) surface

Table 1 The catalytic energy in TS1 and TS2 for seven catalysts

Catalysts	Activation energy (TS1)	Activation energy (TS2)
Fe–N–C	125.04488	75.82297
Co–N–C	147.18699	185.5135
Fe–N ₃ P–C	246.73983	84.72138
Co–N ₃ P–C	232.85531	166.88575
Fe–N ₃ B–C	286.74646	157.66366
Co–N ₃ B–C	232.74383	225.82614
Pt/C	341.38092	206.77598

only single 2p electron of boron atom hybridized with 3d electron of Fe/Co thereby weaker charge density at Fe/Co

atom (e.g., Fig S1). The Pt/C shows homogeneous charge density between atoms.

3.2 Catalytic process

The first single-atom catalyst (SAC) investigated was the Fe–N–C (Fig. 3), in which the –H and –OH produced by H₂O were ordered on carbon and nitrogen atoms, respectively (structure I). The mutual effect between introduced CH₄ and structure (I) led to significant decrease in energy (structure II), which was critical to adsorb fast diffused odor-chemicals with high capacity on surface. The CH₄ in structure II was catalyzed to form –H and –CH₃ bonded with –OH and nitrogen atom, respectively (structure III), the direct Fe–CH₃ interaction (III) resulted from good diffusion capacity on Fe–N–C surface and –CH₃ bonded with

Fig. 4 **a** and **c** CH_4 migration pathways for Fe–N–C and Pt–C. The arrows in the crystal structure represent the CH_4 migration pathway determined from DFT calculations. The red and green arrows indicate path I and II directions, respectively. **b** and **d** Calculated CI-NEB migration barriers for Fe–N–C and Pt–C

low-spin Fe: $t_{2g}^6e^+x$. In fact, Fe– N_4 consumed low activation energy (125.04 kJ/mol) for transition state 1 (TS1). The good catalytic stability along with low O_2 absorbing energy (structure IV), that offered fast diffusion characteristics with good reversibility. With these features, Fe–N–C remained as one of the best single-atom catalysts with a low barrier energy of 75.82 kJ/mol (TS2). The Fe–N–C catalyst solved two major challenges associated with the odor diffusion and carbonization pursued in structure (V). It enabled not only a substantial decrease in the activation energy but also the presentation of a catalyst without the need to employ noble metal Pt. For Pt, a similar catalytic process was calculated (Fig. S2). However, the Pt/C needed the most activation energy as seen in Table 1 and higher diffusion energy in path II (Fig. 4), which led to a release of commercial use from noble metal platinum to non-noble metal iron. Therefore, despite good catalytic performance, practical viability of Pt/C was hampered by the lack of metal platinum that could survive at exploring single metal Fe–N–C materials. Following Fe– N_3P –C and Fe– N_3B –C, the catalytic process has been investigated, and the results were similar with Fe–N–C (Fig. S3–S4).

3.3 Catalytic performance

With an aim to outline the catalytic performance and to develop utility catalysts with non-noble metals (Fe and

Co), six kinds of similar catalysts were explored and compared with Pt/C. The catalytic process was determined by the reaction between active sites with odor (e.g., methane) in air. This mean that catalysts with high performance lie as low as activation energy, which implies that striding saddle points consume as low as possible energy. Therefore, the key is how to access the lower-lying barrier energy of nitrogen and phosphorus or boron dual-coordinated iron or cobalt atoms on supporting carbon materials so that the CH_4 is transformed into H_2O and CO_2 . After a series of calculations for Co/Fe–N/P/B–C and Pt/C catalyzing CH_4 under same environment, the result suggested that noble Pt: $6s^14f^{14}5d^9$ supported by carbon materials consumed high activation energy (341.38 kJ/mol for TS1, 206.78 kJ/mol for TS2) (Table 1). The Fe–N–C resulted in 125.04 kJ/mol for transition state 1 and 75.82 kJ/mol for transition state 2, which was significant decrease relative to Pt/C. The Fe/Co– N_3P –C suffered from higher barrier energy in TS1 than Fe–N–C due to polarization of electrons, so it is inferior corresponding to non-replacing Fe/Co–N–C. The Fe/Co– N_3B –C catalyzed CH_4 at a higher activation energy than Fe/Co– N_3P –C, but it was advantage compared with Pt/C. Overall, all of these Fe/Co single-atom catalysts consumed activation energy of 200.87–458.57 kJ/mol for transition site 1 and 2, the Fe–N–C system displayed the lowest total activation energy of 200.87 kJ/mol. The coordinated effect by the – N_4 and – N_3P or – N_3B group significantly decreased

the activation energy to 89.59–347.29 kJ/mol compared to 548.17 kJ/mol for the single-atom platinum supported on carbon material. These catalysts do have high performance when used to carbonization of odor-chemicals, thereby the similar classes of catalyst could be explored by replacing nitrogen with phosphorus and boron elements.

To evaluate and understand the CH₄ migration mechanisms and pathways, we calculated the CH₄ bond-valence site energy using the BVSE method and the single CH₄ migration barriers using the CI-NEB method. Figure 4a, c showed the migration pathways of CH₄ in path I and II, respectively. The energy barriers for Fe–N–C in path I and path II were 0.0087 and 0.0099 eV, respectively. The calculated energy barrier for Pt/C in path I (0.0067 eV) was lower than path II (0.0103 eV). These migration barriers were less than or equal to 0.01 eV in path I and path II, indicating that fairly good migrate and storage capacity can be expected in these catalysts (Fig. 4b, d).

4 Conclusion

In this work, Vienna ab initio simulation package (VASP) with density functional theory method was employed as a means to explore catalytic performance and process, activity sites, stability and storage capacity of Fe/Co–N/P/B–C for removing odor-chemicals of cooking source. According to catalytic performance, Fe/Co–N/P/B–C was found to be preferred than Pt/C. In the superior case of carbonizing CH₄ corresponding to Fe–N–C, CH₄ was absorbed at the (001) surface, on which –H and –OH were ordered at N activity site and C atom, respectively. And following, CH₄ was transformed to –H and –CH₃ that was linked with iron activity site. Finally, the –CH₃ was oxidized to C and H₂O. In this case, energy barrier 1 and 2 were 125.04 and 75.82 kJ/mol, which were lower 216.33 and 130.95 kJ/mol than Pt/C, respectively. Meanwhile, diffusion energy of CH₄ on Fe–N–C (001) surface was close to Pt/C through path I and II, which suggested that Fe–N–C had the similar storage capability with Pt/C. Moreover, based on the quantitative study of charge density and projected density-of-states (PDOS), we have clearly shown evidence that 3d electrons in Fe/Co–N/P–C are the predominant factor determining stability. In addition, the large charge density around Fe/Co atom and overlap between Fe/Co: 3d and N: 2p/P: 3p orbitals above the Fermi level play crucial roles in activity sites. We expect more exciting studies on diverse single-atom catalysts or other kinds of catalysts in a theory & experiment method.

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Compliance with ethical standards

Conflict of interest The author declares no competing financial interest.

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