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Hydrogen storage mechanisms in defective graphenes

Utkir Uljayev

utkir.uljaev@outlook.com

Kamoliddin Mehmonov
Ishmumin Yadgarov
Maksudbek Yusupov
Umedjon Khalilov

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Abstract

Research on hydrogen storage using carbon-based nanomaterials is currently attracting increasing interest. Yet, understanding the storage nature of graphene surfaces is still elusive. In this study, we investigated the physisorption mechanisms of H2 molecules on defective graphenes using reactive molecular dynamics simulations. We found that an increase in the size and concentration of defects in graphene increases the physisorption of H2 molecules on the surface due to a change in the partial charges of atoms in the system. Specifically, our results showed that in the case of the highest percentage of defects (10.27%), the gravimetric density of H2 molecules is about 2.12 wt.% at ambient conditions, which is within the range of gravimetric densities obtained from experiments and other simulations. The results also indicated that the physisorption of H2 molecules is related to both the size and the concentration of defects on the graphene surface. This study contributes to a better understanding of the mechanisms of hydrogen storage in graphene with various defects at the atomic level.

INTRODUCTION

Hydrogen energy is considered a highly promising “green” fuel in various fields, such as fuel cells [1,2], electronics industry and pharmaceuticals, due to its environmentally friendly and sustainable nature. It is predicted to be an efficient alternative fuel that can be used to generate energy. Currently, research is being carried out on the process of extracting (or producing) hydrogen from water using photocatalytic and electrocatalytic decomposition methods [3,4]. Hydrogen production methods have been extensively studied in various countries. Specifically, in Japan, efficient catalysts such as TiO_2 (anode) and SiC (cathode) are used to extract hydrogen [5], whereas in Spain, a project utilizing photoelectrocatalysis was launched to produce fuel from hydrogen [6]. Australia is also producing hydrogen using solar and wind energy [7]. Hydrogen can also be extracted at high temperatures from various compounds and molecules [8], including methane, using nanomaterials [9,10]. Recently, attention has been drawn to the regenerative method of hydrogen production in a plasma reactor, which is being studied theoretically and practically [11].

Hydrogen extracted from various sources is being extensively used as a source of energy in various technologies and industries. Russian company NOVATEK has significantly increased the use of hydrogen in its steam-gas plants, with a share of 60%, and launched the first industrial project to generate electricity from it [6]. Meanwhile, at the port of Tallinn in Estonia, ferries use hydrogen, which is known to be an environmentally friendly fuel [12]. About 300 households in Scotland have begun the transition from natural gas to clean hydrogen [13]. Apple in the US recently began developing a hydrogen fuel cell-using mobile device for testing under controlled laboratory conditions [14]. In addition, France has successfully engineered aircrafts that are powered by hydrogen engines [15,16].

To ensure the efficacy of hydrogen energy, it is crucial to adequately store the isolated hydrogen in materials [17-20]. Hydrogen can be stored using three primary methods, i.e., compressed gas [21],

cryogenic liquid [22] and solid storage [23]. The solid state storage method is considered safer and more economical than the other two methods due to the absorption of hydrogen by the nanomaterials, which reduces the large volume and additional energy required. Currently, research is being conducted using metal hydrides [24], complex hydrides [23] and carbon-based nanostructures [25,26] as hydrogen storage materials. Particular attention is paid to both physisorption [27] and chemisorption [28] methods of hydrogen storage in these materials and consistent efforts are being made to study their effectiveness. Recently, there has been increased interest in carbon-based nanomaterials that have a high hydrogen storage index. Because of their chemical stability and large storage capacity, these nanomaterials are considered good candidates for effective hydrogen storage [29]. In particular, graphene [30], one of the carbon-based nanomaterials, is being considered as a promising material for hydrogen storage due to its high mechanical, chemical, electrical, optical and thermal properties [31]. Hydrogen atoms and molecules can be adsorbed on both sides of graphene, which increases its storage capacity [32]. Although studies have been carried out on hydrogen storage using physisorption and chemisorption in one and two layers of defect-free and defective graphene structures, the actual storage efficiency at room temperature remains low. Nevertheless, theoretical studies continue to explore ways to improve this performance [33,34]. Recent studies have shown that graphene with defects (such as a single Stone-Wales vacancy or a double vacancy, i.e. 5-8-5, 555-777 and 5555-6-7777) has a higher hydrogen storage capacity compared to defect-free graphene [35,36]. This finding highlights the potential for utilizing defective graphene in hydrogen storage applications [35]. Despite various attempts, the ability of graphene to store hydrogen on its surface is still limited due to the diverse range of defects in its structure, which differ in type and size.

In this research, we investigate the underlying mechanisms of hydrogen adsorption on graphenes with and without defects using atomistic computer simulations, in order to understand how to improve the hydrogen storage capacity of carbon-based nanomaterials.

COMPUTATIONAL DETAILS

We performed the reactive molecular dynamics (MD) simulations using the LAMMPS software package [37] to simulate the adsorption processes of H_2 molecules on various graphene surfaces, including defect-free and defective ones. For this purpose, we used the ReaxFF potential with a parameter set developed by Zou et al. [38], to accurately describe the interatomic interactions, including the formation and breaking of chemical bonds between them. As model systems, we used different graphene structures, i.e., pristine graphene (*G*) (Fig. 1a) and graphene with single (*SVG*), double (*DVG*) and triple (*TVG*) defects (Fig. 1b-g). To determine the percentage of defects in graphene, the ratio of the surface area of defective (*SVG*, *DVG* and *TVG*) graphenes $S_{dG}= S_{SVG}+ S_{DVG}+ S_{TVG}$ was divided by the surface area of pristine graphene S_G, resulting in the value $k=S_{dG}/S_G$. This value was used to analyze the impact of defects on the graphene structures. Thus, according to this formula, the *k* coefficients of graphenes with one (k_{SVG}), two (k_{DVG}) and three (k_{TVG}) defects were determined as $k_{SVG}= S_{SVG}/S_G$, $k_{DVG}= S_{DVG}/S_G$ and $k_{TVG}= S_{TVG}/S_G$, respectively. As shown in Figure 1b-g, the number of defects used in this study for

defective graphene was chosen to be 1 (*SVG-1, DVG-1* and *TVG-1*) and 4 (*SVG-4, DVG-4* and *TVG-4*). To calculate the overall percentage of defects (or their concentration) on the graphene surfaces, the individual percentages of defects on *SVG, DVG* and *TVG* were added together: $k=k_{SVG}+k_{DVG}+k_{TVG}$. The measured surface area of *G* graphene was 10.18 nm^2 while the surface area of defects, i.e., *SVG-1*, *DVG-1*, *TVG-1*, *SVG-4*, *DVG-4* and *TVG-4*, on defective graphene was found to be 0.16, 0.21, 0.26, 0.63, 0.84 and 1.05 nm^2, respectively. Thus, the *k* coefficients (or percentages of defects) of these *SVG-1*, *DVG-1*, *TVG-1*, *SVG-4*, *DVG-4* and *TVG-4* graphenes were 1.54, 2.05, 2.57, 6.15, 8.22 and 10.27%, respectively.

Thus, seven model graphenes were used in total, i.e., *G*, *SVG-1*, *DVG-1*, *TVG-1*, *SVG-4*, *DVG-4* and *TVG-4*. First, the potential energy of these model systems was minimized using the conjugate gradient method. Subsequently, they were heated up to 300 K using an *NpT* ensemble and a temperature gradient of 1 $K \bullet ps^{-1}$ [39], applying the Berendsen thermostat and barostat with coupling constants of 100 fs and 5000 fs, respectively [40]. Then, the temperature of the model systems (300 K) was controlled using a Bussy thermostat in the *NVT* ensemble [41] for 100 ps. To mimic infinitely long systems, the model graphenes were subjected to periodic boundary conditions in both the *x* and *y* directions.

In the simulations, the pressure of H_2 molecules in the system is calculated as $p = J\sqrt{2\pi MRT}/N_A$, where J – impingement flux ($nm^{-2} \cdot ns^{-1}$), N_A – Avagadro's number, R – universal gas constant, M – a molar mass ($kg \cdot mol^{-1}$) of H_2 molecule and T – temperature of the system (K). During the *NVT* simulations, H_2 molecules were introduced into the environment surrounding the graphene surface (10.18 nm^2) at a time interval of 10 ps. The distance between each introduced H_2 molecule and the model system was chosen to be at least 12 Å (i.e., the cut-off radius of the interaction potential). Under these conditions, the impingement flux of the incident H_2 gas was 9.82 $nm^{-2} \cdot ns^{-1}$ and its corresponding pressure was 91.28 kPa (i.e., 0.90 atm). The concentration of physisorbed H_2 molecules on the graphene surface was calculated as the gravimetric density, i.e., $wt.\% = (1 + m_C N/m_H n)^{-1} \times 100\%$, where m_C and N (m_H and n) are the mass and number of carbon (hydrogen) atoms. In all MD simulations, a time step of 0.1 fs was used for a total simulation time of 3 ns. The simulations were repeated at least 5 times for each study case, and the final results were obtained by averaging the individual physical quantities.

RESULTS AND DISCUSSION

As an example of the hydrogenation process of graphene, figure 2 illustrates the defective graphene *TVG-4* (i.e., graphene with the highest concentration of defects in this work) and surrounding H_2 molecules. It was suggested that nanostructures based on carbon nanomaterials (graphene, nanotubes, etc.) can exhibit physisorption of H_2 molecules in close proximity to the nanostructure, i.e., in the range of 3 Å [42]. Therefore, we used a cut-off distance of 3 Å from the graphene surface to determine the amount (or concentration) of physisorbed H_2 molecules. As is obvious, a greater number of H_2 molecules (i.e., 42% of the total H_2 molecules in the system) within 3 Å of the surface are physisorbed on *TVG-4* graphene (see Fig. 2).

The reactivity of carbon-based nanostructures such as fullerene, nanotubes and graphene is mainly determined by the significant mechanical pressure that occurs due to the spherical shape caused by carbon atoms, which can be identified by the pyramidalization angle (θ_p) [43]. The curvature of *p*-orbitals in carbon nanotubes (CNTs) causes local strain (or deformation), leading to pyramidalization and displacement of C atoms. Consequently, this strain can increase reactivity in CNTs due to an increase in their curvature. On the other hand, the reactivity in flat graphene sheets is considerably low, since C atoms have sp^2 hybridization in a planar form with a zero pyramidalization angle. (θ_p=0°). Thus, the interaction of H_2 molecules with the graphene surface most likely has a physisorption character.

Figure 3 shows the gravimetric density of physisorbed H_2 molecules, depending on the concentration of defects (see red curve). As is clear, the concentration of defects ranges from 0 to 10.27%, i.e., from defectless graphene (*G*) to highly defective one (*TVG-4*). It is obvious from the figure that the gravimetric density of H_2 molecules physisorbed on *G* graphene is 1.56 wt.%, which increases with an increase in the number (concentration) of defects on graphene, thereby reaching a value of 2.12 wt.% for *TVG-4*, i.e., highest defectiveness. For other defects, the gravimetric density is found to be 1.76, 1.88, 2.01, 2.06 and 2.08 wt.% for *SVG-1*, *DVG-1*, *TVG-1*, *SVG-4* and *DVG-4*, respectively. These values are within the range of gravimetric densities obtained using MD simulations 2.0-2.20 wt.% [36], respectively. In general, at 300 K, the amount of hydrogen covering the surface (represented as N_H/N_C) is around 18.75% for pristine graphene. However, in the case of graphenes with concentrations of defects within the range of 1.54-10.27%, the degree of hydrogen coverage also differs, reaching a maximum value of 25.74%. This means that with an increase in the concentration of defects in graphene, the number of H_2 molecules that can adsorb to its surface also increases. The increase in the gravimetric density of physisorbed H_2 molecules on the graphene surface with an increase in the concentration of defects can be explained by the change in the partial charges of C atoms (see Fig. 3, blue curve). In graphene, the carbon atom has a higher electronegativity value (χ=2.55) compared to the hydrogen atom (χ=2.20). This difference in electronegativity results in non-bonded interactions such as Van der Waals and Coulomb forces between the graphene surface and H_2 molecules. As a result, the average partial charge of C atoms in graphene is -0.121, -0.124, -0.136, -0.188, -0.192 and -0.201*e*, which corresponds to the values of 1.54, 2.05, 2.57, 6.15, 8.22 and 10.27% of the defect concentration in graphene. This indicates that an increase in the concentration of defects leads to an increase in the partial charges of C atoms in defective graphenes. This, in turn, results in a relatively stronger interaction between H_2 molecules and C atoms on the graphene surface, thereby leading to higher adsorption of H_2 molecules on defective graphene.

Figure 3 (red curve) also shows that the rate of hydrogen adsorption sharply increases with an increase in the size of defects at a lower concentration. In particular, the average rate is 0.175 wt.% on the percentage of defects for *SVG-1*, *DVG-1* and *TVG-1*. However, this rate decreases by about 12 times for the cases of *SVG-4*, *DVG-4* and *TVG-4*, i.e., with an increase in the size of defects while maintaining their higher concentration. Nevertheless, it can be assumed that even at low concentrations, an increase in the size of defects can most likely lead to a decrease in the adsorption rate due to the formation of

larger voids and, as a consequence, the weakening of non-bonded interactions between H_2 molecules and defective graphene. Indeed, the use of smaller defects instead of larger ones, at the same concentration of defects, can lead to a higher degree of retention of H_2 molecules on the graphene surface [44]. Note that there is a limitation on the concentration of defects, under which an excessive number of defects can lead to the opposite results on the hydrogen adsorption rate [45], which can be caused by the formation of larger defects (voids) due to the clustering of smaller-sized defects [46,47].

CONCLUSIONS

Molecular dynamics simulations were performed to study the physisorption of H_2 molecules on defective graphenes with various defect sizes compared with pristine graphene. The results showed that an increase in the size and concentration of defects in graphene leads to an increase in the physisorption of H_2 molecules on the surface, which is associated with an increase in the partial charges of C atoms and, consequently, a stronger non-bonded interaction of H_2 molecules and C atoms on graphene. In particular, for the case of the highest percentage of defects (10.27%), the gravimetric density of H_2 molecules was found to be 2.12 wt.% at 0.9 atm and 300 K. Overall, the physisorption nature (in particular, adsorption rate) of H_2 molecules depends on both the size and the concentration of defects on the graphene surface.

In general, this study helps to understand the underlying mechanisms of hydrogen physisorption on defective graphenes, which in turn improves our understanding of how to manipulate defects in order to increase the hydrogen storage capacity.

Declarations

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Figures

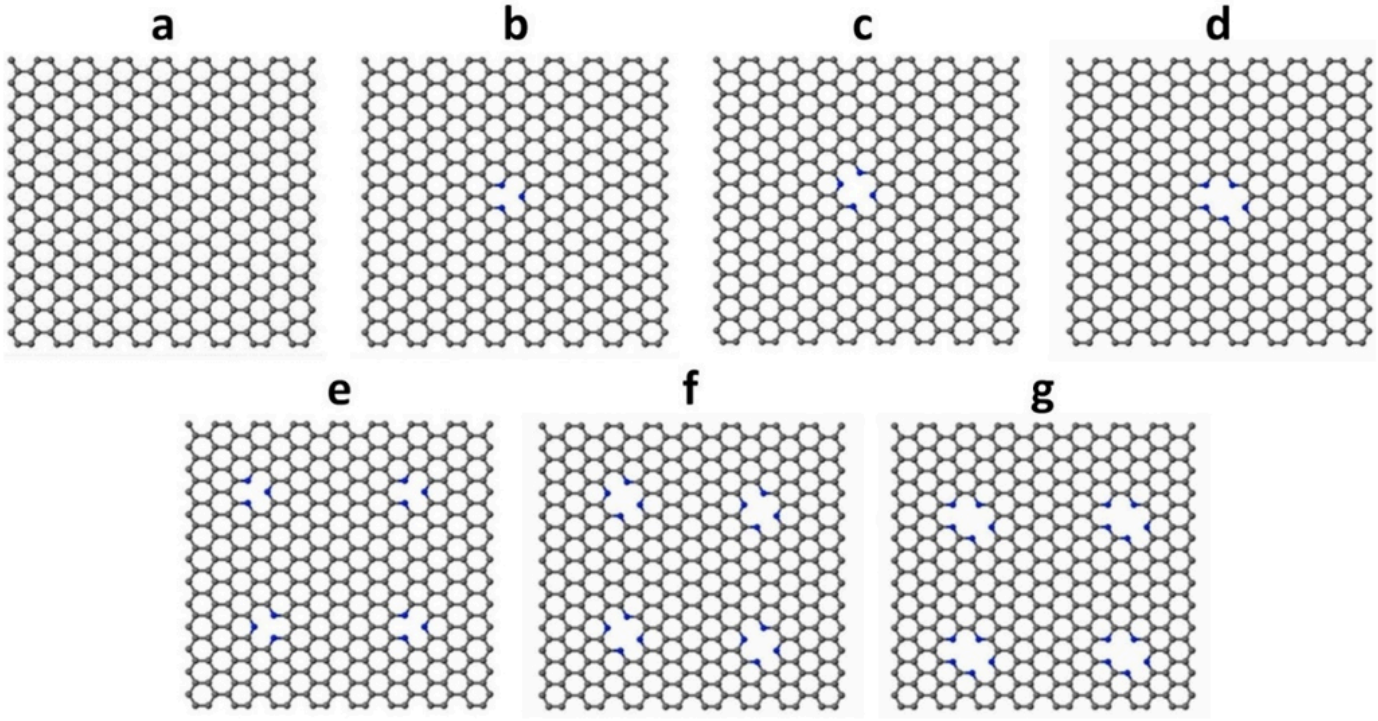


Figure 1

Defect-free (pristine) graphene G (a) and defective graphenes with different concentrations, i.e., SVG-1 (b), DVG-1 (c), TVG-1 (d), SVG-4 (e), DVG-4 (f), TVG-4 (g). The numbers denote one (b-d) or four (e-g) defects in the defective graphene.

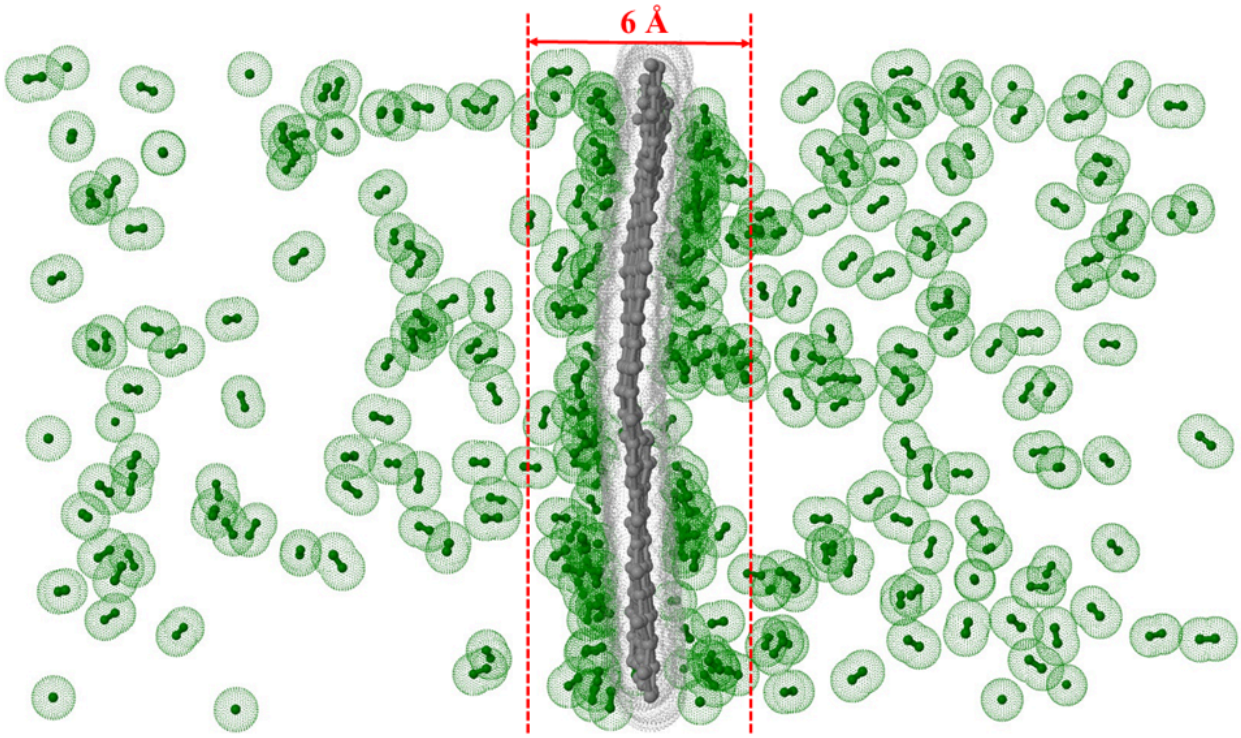


Figure 2

Cross section of graphene with surrounding H_2 molecules. H and C atoms with Van der Waals spheres are shown in green and gray colors, respectively. A cut-off distance of 3 Å is chosen for physisorption.

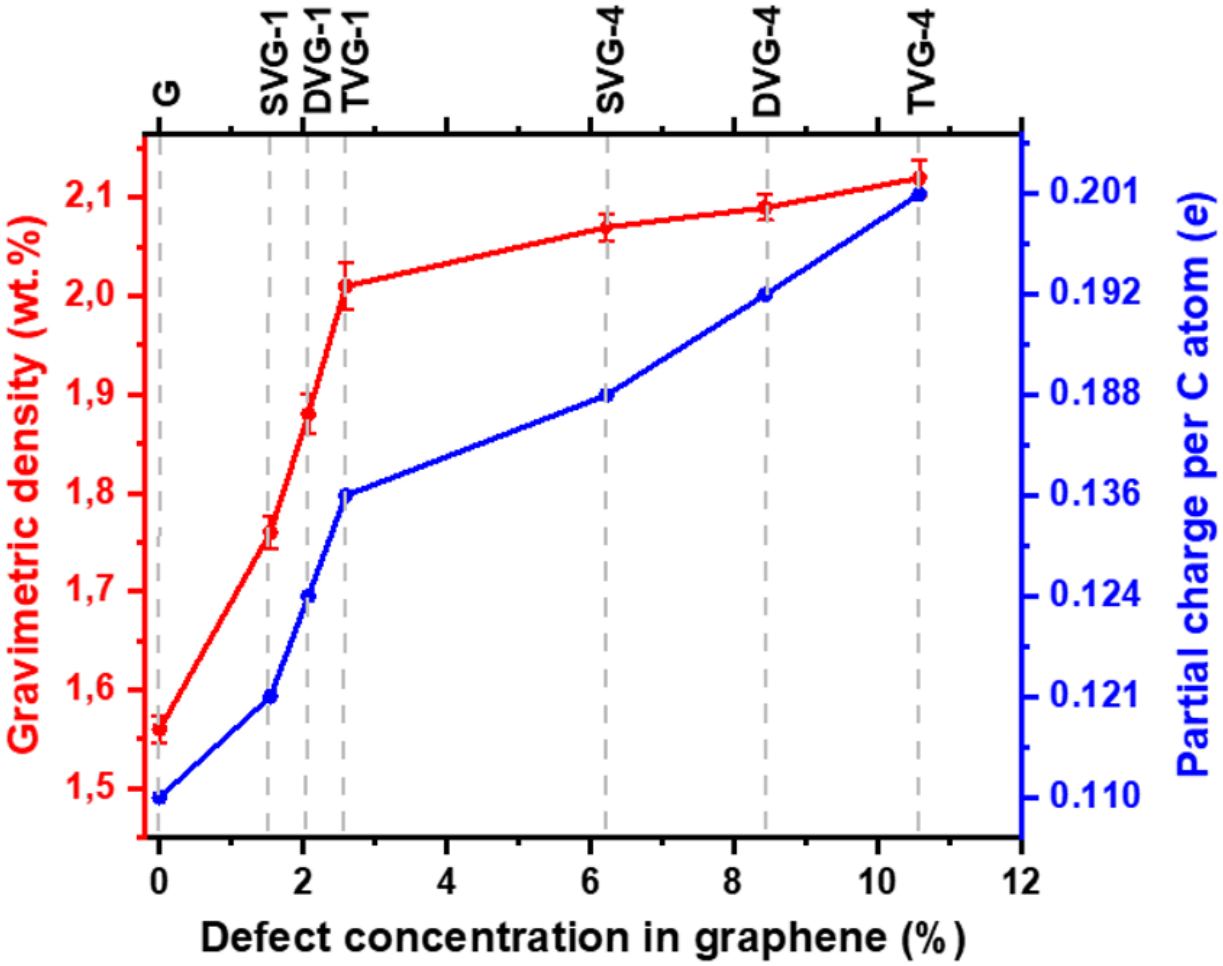


Figure 3

The average gravimetric density of physisorbed H_2 molecules (left, red curve) and the average partial charge of C atoms in graphene (right, blue curve), depending on the concentration of defects.