Graphene oxide and adsorption of chloroform: a density functional study

Elena Kuisma, C. Fredrik Hansson, Th. Benjamin Lindberg, Christoffer A. Gillberg, Sebastian Idh, and Elsebeth Schröder

Quantum Device Physics Laboratory, Microtechnology and Nanoscience (MC2), Chalmers University of Technology, SE-412 96 Göteborg, Sweden

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Chlorinated hydrocarbon compounds are of environmental concerns, since they are toxic to humans and other mammals, are widespread, and exposure is hard to avoid. Understanding and improving methods to reduce the amount of the substances is important. We present an atomic-scale calculational study of the adsorption of chlorine-based substance chloroform (CHCl$_3$) on graphene oxide, as a step in estimating the capacity of graphene oxide for filtering out such substances, e.g., from drinking water. The calculations are based on density functional theory (DFT), and the recently developed consistent-exchange functional for the van der Waals density-functional method (vdW-DF-cx) is employed. We obtain values of the chloroform adsorption energy varying from roughly 0.2 to 0.4 eV per molecule. This is comparable to previously found results for chloroform adsorbed directly on clean graphene, using similar calculations. In a wet environment, like filters for drinking water, the graphene will not stay clean and will likely oxidize, and thus adsorption onto graphene oxide, rather than clean graphene, is a more relevant process to study.

Keywords: graphene oxide, chloroform, vdW-DF, vdW-DF-cx, van der Waals, DFT, adsorption, water filtering, water cleaning

I. INTRODUCTION

Graphene oxide was first synthesized more than 150 years ago, but caught general interest only during the past few decades when research in 2D materials, in particular graphene, has started to bloom. Graphene oxide is an alternative path to large-scale production of graphene, by liquid-phase exfoliation of graphite oxide into layers, called graphene oxide (GO), and subsequent reduction to graphene, but already the GO sheets have intriguing and useful features. GO can be understood as functionalized graphene, oxidized with hydroxyl, epoxide and some carboxyl groups. Its properties depend on the details of the oxidation: the type of, the number of and the distribution of the functional groups. GO has tuneable electric properties, obtained by changing the functional groups, and with its thin size could be used for electronics. GO is highly catalytic, highly solvable in water and other solvents, and is proposed for use as a gas sensor.

GO has been suggested as a material for use in filtering of toxic compounds such as chlorinated hydrocarbon compounds. These are some of today’s environmental concerns, since they are toxic to both humans and other mammals, and exposure is hard to avoid. Exposure to chlorine-based compounds arises, e.g., from consumption of chlorinated drinking water or food supplies that have been contaminated by residues of industrial chemicals. Therefore we here use the van der Waals (vdW) density functional method (vdW-DF), in the vdW-DF-cx version, for all calculations except for a comparison with previous results, where we use PBE for some calculations.

Chloroform with graphitic or other carbon based materials was previously studied in a couple of experimental and computational studies. A DFT based study of ammonia adsorption was presented earlier. However, to our knowledge there are no previously DFT studies of chloroform physisorption on GO using methods that include the vdW interactions consistently, such as here. Certainly, physisorption of chloroform on GO with the recent vdW-DF-cx has not previously been covered.

This article is structured as follows: In Section II we describe the method of computation and the systems studied. In Section III the results are presented and discussed, along with a discussion of the accuracy of our calculations, and Section IV summarizes the study.

II. PHYSICAL SYSTEM AND COMPUTATIONAL METHOD

In the following we describe GO and its functional groups and how we model the relevant parts of GO in our adsorption study. We also describe the methods used for
the DFT calculations and define the binding energies for the functional groups in GO and for chloroform on GO, including a discussion of what constitutes the zero point of the binding energies in these calculations. This varies in the literature, making comparison difficult.

**A. GO and chloroform**

GO has a graphene carbon network with an almost amorphous distribution of functional groups, and it is difficult to determine the types of functional groups present and their positions. In Ref. 6 Lerf et al. used reactions with various reagents to supplement their previous NMR measurements. They found that graphite oxide (and thus likely also GO) mainly has two types of functional groups: O bound in the C-C bridge site, which is the 1,2-ether or epoxide, and the C-OH or hydroxyl group. They also found no support for O bound to two next-nearest neighbor C atoms (the 1,3-ether) and very little for the carboxyl (the -COOH) group. Based on their measurements they put forward a structural model for GO that has areas without functional groups (i.e., areas of clean graphene) and other areas with epoxide and hydroxyl groups randomly distributed but close together. In their model the carbon grid of GO is almost flat, except for the parts where C atoms are attached to hydroxyl. The GO has functional groups on both sides of the carbon grid and carboxyl groups are only present at the edges of GO.

In experiments, fully oxidized GO is found to have a C:O ratio approximately 2:1 or more. However, GO is not always found in the fully oxidized state. Even though the GO model of Lerf et al. has a relatively high concentration of functional groups, the C:O ratio is only about 5:1 in the areas that are not part of the GO sheet edges.

In the present study of GO we consider structures with clusters of functional groups on otherwise clean graphene, the clusters being relatively small and disordered. Thus, we compute the structures and energies involved in the formation of epoxide and hydroxyl groups on graphene for GO with low O concentration (C:O ratio from 72:1 to 15:1). We use GO with functional groups on either both sides of the carbon grid (not symmetrically positioned) or one side with just a few clustered groups only. In our study we use periodic boundary conditions in space and thus the GO has no edges. This means that according to the model by Lerf et al. there should not be any carboxyl groups included.

Chloroform (CHCl₃) consists of a central carbon atom with three electro-negative Cl atoms in a ‘tripod’ in one end and a H atom at the other end. This gives chloroform a finite dipole moment, which affects its physisorption properties.

In our chloroform adsorption study we initially studied mainly (but not exclusively) GO structures that have all functional groups on the same side as the adsorbed molecule because these groups were supposedly the ones that influence the chloroform-GO binding the most. However, we see that also groups on the other side of the carbon grid affect the adsorption energy and our study has been enlarged to enclose also systems with functional groups on both sides.

**B. Unit cell**

To study GO we start out with a graphene slab with added functional epoxide and hydroxyl groups. We use a $3\sqrt{3} \times 6$ orthorhombic unit cell with 72 graphene C atoms, as illustrated in Figure 1 with a C-C distance of 1.424 Å, and periodic boundary conditions. The unit cell height is varied such that the amount of vacuum between each copy of the system is approximately 10 Å, thus for clean GO calculations the unit cell height is 10.5 Å, and approximately 15.5 Å for physisorption of chloroform on GO. In the calculations of adsorbed chloroform the molecule-molecule nearest-neighbor distance is 12.8 Å (the unit cell width) and the smallest lateral distance between any two atoms in neighboring chloroform molecules is 10.4 Å, as illustrated in Figure 2.

**C. Methods of computation**

The formation of GO from graphene is a process in which hydroxyl and epoxide groups chemisorb on graphene. Such processes are expected to be well described with a semilocal density functional like PBE. However, the adsorption of chloroform on GO is a physisorption process and in such processes a robust de-
The size of the unit cell (white box) is approximately 12.8 × 14.8 × 15.5 Å. Color legend: Chloroform has yellow C; lime Cl; blue H, and GO has gray C; red O. Closest atom-atom distances between chloroform molecules are indicated, $d_1 = 10.4$ Å and $d_2 = 11.9$ Å. Visualization using VMD.

FIG. 2. Sketch of the unit cell used for calculations of chloroform adsorption on GO. The size of the unit cell (white box) is approximately 12.8 × 14.8 × 15.5 Å. Color legend: Chloroform has yellow C; lime Cl; blue H, and GO has gray C; red O. Closest atom-atom distances between chloroform molecules are indicated, $d_1 = 10.4$ Å and $d_2 = 11.9$ Å. Visualization using VMD.

The phase transition between diamond and graphite, $sp^3$ and $sp^2$ materials, is encouraging. To further document the ability of vdW-DF-cx for this problem we compare formation energies for a number of unsaturated GO configurations, obtained with both the vdW-DF-cx and the semilocal PBE functional.

For the vdW-DF-cx results and most of the PBE results we use Quantum Espresso (QE). For further comparison we perform additional PBE calculations using the GPAW software. All calculations are carried out self-consistently.

In the QE calculations we use ultrasoft pseudopotentials with wavefunction and density cut-off energies 30 and 120 Ry, respectively. The force convergence threshold value is set to 2 meV Å$^{-1}$, and the number of k-points is $4 \times 4 \times 1$ (and $1 \times 1 \times 1$ for small molecules). With GPAW we use PAW setups in the GPAW standard.

The binding energy of the functional groups on graphene and of chloroform on GO, is calculated as

$$E_b = -(E_{AB} - E_A - E_B),$$

where $E_{AB}$ is the total energy of the full system and $E_A$ and $E_B$ are the total energies of its individual constituents (positive $E_b$ for systems that bind). The zero point for the binding energy depends on the choice of individual constituents in subsystem A and B, e.g., whether to use an isolated O atom or the $O_2$ molecule as one of the subsystems. These choices vary among authors of such studies. Our choice is discussed below.

Spin polarization was not implemented in vdW-DF-cx at the time of our calculations, and thus we approximate the binding energy of an epoxide on graphene as

$$E_b^{cx} = -(E_{GO}^{cx} - E_G^{cx} - E_O^{cx}),$$

$$\approx -(E_{GO}^{cx} - E_G^{cx} - (E_{O}^{PBE} - E_{iO}^{PBE} + E_i^{cx})), \quad (3)$$

where $E_{GO}$ and $E_G$ are the total energies of GO and graphene, and $E_O$ and $E_{iO}$ are the energies of triplet ($^3O$) and singlet ($^1O$) O atoms, respectively, and the superscript denotes the functional used, vdW-DF-cx or PBE. Thus, the difference in O singlet and triplet total energy in vdW-DF-cx is approximated by the same difference in PBE, $E_{O}^{PBE} - E_{iO}^{PBE} \approx E_{O}^{cx} - E_{iO}^{cx}$. The binding energies of the hydroxyl groups are calculated in a similar manner, whereas the chloroform-on-GO calculations are carried out without considering spin, with a non-spinpolarized calculation of chloroform and a graphene calculation as the two individual constituents.

In the results section we report the height $h$ of the chloroform molecule above GO in the adsorbed position. The height is taken as the projection in the $z$-direction (i.e., perpendicular to graphene) of the distance between the chloroform C atom and the nearest GO surface O atom. This means that an atom in chloroform may be closer to the GO O-atom than the distance $h$.

III. RESULTS AND DISCUSSION

A. Oxidized graphene

We focus on lightly oxidized graphene, with only a few functional groups per 72 C-atom unit cell. We use 10
different configurations with up to three epoxide groups and up to two hydroxyl groups per unit cell, as illustrated in the left hand side of Figure 3. The functional groups are placed such that they form clusters, as expected from experiments. The resulting binding energies are presented in the graph on the right hand side and in Table I. Structures GO1–3 and GO6–9 have groups on one side of the graphene plane only, structures GO4–5 have one epoxide on each side, and structure GO10 has epoxide and hydroxyl groups on both sides. The C–O lengths for the epoxides and hydroxyl groups are 1.47 Å and 1.52 Å with the vdW-DF-cx functional.

By studying the binding energy $E_b$ for each structure we find that $E_b$ has an almost linear dependence on number of C atoms involved in binding the functional groups: the right hand side of Figure 3 shows that for every C atom involved (meaning there will be one less sp$^2$-bound C atom) $E_b$ increases by roughly 1.5 eV. For comparison, one single hydroxyl group has a binding energy of about 1 eV and the epoxide group, with its two C-O bonds, has a binding energy of about 2.3 eV, so the gain in adding a functional group to a cluster is significantly higher, per C-O bond, than just adding the group to a patch of clean graphene. There is some spread in the numbers, and the illustrations of the structures show that the clusters of functional groups are not all densely packed, leading to less gain in energy for sparse clusters than for more dense clusters.

The preference for having functional groups in clusters is seen already in a cluster of two hydroxyl groups: we see a huge gain in energy (almost 1 eV) by pairing hydroxyl groups, instead of having them separated. This is so even when the groups are on the same side of the graphene grid and give rise to more distortion of the graphene than the distortion created by one single hydroxyl group (structure GO6 compared to GO2 times 2).

More generally, by visually comparing all of the structures in the left hand side of Figure 3 we find that structures with groups on both sides (GO4, GO5, and GO10) have a less distorted carbon structure than structures with groups only on one side (all others), as expected.

Table I shows that for structures with two epoxides (GO3, GO4, and GO5) an energy gain can be obtained both by clustering, with gain per O atom 0.36 eV (from comparing GO1 and GO4), and by having the epoxide groups on both sides of the graphene instead of one side (gain 0.11 eV) but also that the largest gain is obtained by having the epoxides as nearest neighbors as opposed to next-nearest neighbors (gain 1.21 eV). This is seen independent of DFT method (vdW-DF-cx and PBE) and computational code (QE and GPAW) and can also be seen in literature values.

Returning to the full set of formation energy results, Table I, we can compare the results of PBE calculations to vdW-DF-cx calculations. The PBE calculations are expected to get both the sp$^2$ and sp$^3$ binding of the C atoms reasonably correct (but not so for the long-range interactions, which are important in chloroform physisorption). We find that the vdW-DF-cx formation energies are systematically stronger than those of PBE, with up to 23% difference in formation energies. However, the difference depends on the type of functional group(s) involved in the GO structure: for epoxides the difference in formation energy of vdW-DF-cx compared to PBE is 7–9%, whereas the difference is 16–23% for hydroxyl groups, and mixed structures in the range 9–13%.

It is important to note that these differences in vdW-DF-cx and PBE formation energies include changes to the positions of the atoms when changing functional between vdW-DF-cx and PBE and subsequently structurally relaxing the atomic positions. The hydroxyl functional group has an H atom pointing away from graphene, this makes long-range interactions more relevant for hydroxyl that for the epoxide. The single-bonded H atom also has a less stiff binding, and small changes in the forces on the atoms (from change of functional) can more easily move the H atoms than the more stiffly bound O atoms. These differences between the hydroxyl and epoxide functional groups are likely at least part of the reason for the larger PBE to vdW-DF-cx energy difference when hydroxyl groups are involved: vdW-DF-cx may actually turn out to describe those groups better than PBE! However, without experiments or high-quality quantum chemistry calculations to compare to we cannot claim that this is the case.

### B. Adsorption of chloroform

The main goal is to examine how chloroform binds to GO. Our focus is on studying the effect on the binding energy of the presence of and the positions of the epoxide and hydroxyl groups and the relative orientation of the chloroform molecule. Since GO is almost amorphous an exhaustive search is prohibitive. Instead only the few functional groups closest to the chloroform molecule are examined, keeping the rest of the unit cell clean of func-

| GO# | GO struct. | $E_b^{\text{cx}}$ | $E_b^{\text{cx}}/\text{O}$ | $E_b^{\text{PBE}}$ | $E_b^{\text{PBE}}/\text{O}$ |
|-----|-------------|-------------------|--------------------------|-------------------|--------------------------|
| GO1 | O           | 2.341             | 2.341                    | 2.166             | 2.166                    |
| GO2 | OH          | 0.996             | 0.996                    | 0.769             | 0.769                    |
| GO3 | 2O          | 5.187             | 2.594                    | 4.844             | 2.422                    |
| GO4 | 2O          | 5.301             | 2.652                    | 4.937             | 2.469                    |
| GO5 | 2O          | 4.190             | 2.095                    | 3.831             | 1.916                    |
| GO6 | 2OH         | 2.956             | 1.478                    | 2.495             | 1.247                    |
| GO7 | 2O, OH      | 6.620             | 2.207                    | 6.042             | 2.014                    |
| GO8 | O, 2OH      | 4.835             | 1.612                    | 4.189             | 1.396                    |
| GO9 | 3O, 2OH     | 10.583            | 2.117                    | 9.592             | 1.918                    |
| GO10| 3O, 2OH     | 11.462            | 2.292                    | 10.412            | 2.083                    |
TABLE II. Binding energies \( E_b \) and energy differences for GO structures with two epoxide groups, systems GO3, GO4 and GO5 and a single epoxide group, GO1. Calculations performed using QE and GPAW with the vdW-DF-cx and PBE functionals. The structures differ by having epoxide on one (GO3) or both sides (GO4) of the graphene plane, and by having the epoxides placed as nearest neighbors (GO4) or across the graphene carbon ring (GO5). The literature values (Ref. 46) are for similar but not identical systems. All energies in units of eV.

| Structure | This work | This work | This work | This work | This work |
|-----------|-----------|-----------|-----------|-----------|-----------|
|           | QE  vDW-DF | QE  PBE   | GPAW PBE  | GPAW PBE  | GPAW PBE  |
| GO3       | 5.19      | 4.84      |           |           |           |
| GO4       | 5.30      | 4.94      | 5.15      | 4.76      |           |
| GO5       | 4.19      | 3.83      | 4.00      | 3.59      |           |
| GO4-GO3   | 0.11      | 0.10      |           |           |           |
| GO4-GO5   | 1.21      | 1.11      | 1.15      | 1.17      |           |
| GO4-2×GO1 | 0.72      | 0.61      |           |           |           |

Overall the adsorption energy lies approximately in the range 0.2–0.4 eV. A closer look on the various adsorption systems compared for similarities yields the following insights: I compared to II shows that adsorption close to an (isolated) epoxide is more favorable by about 0.08 eV that adsorption close to (isolated) hydroxyl. The systems III, IV, and V compared to I show that adsorption close to a pair of epoxides is more favorable than adsorption on a single epoxide. The gain depends on the relative positions of the epoxides, whether they are on the same side of the graphene plane (III and V) or not (IV), and whether the epoxides are in nearest-neighbor positions (III) or sit across the C 6-ring (V). Placing the epoxides on both sides of the graphene plane shows to be more favorable by about 0.11 eV.

Systems VI and VII are used to examine the dependence on the relative positions of hydroxyl pairs: in these calculations positioning the hydroxyl pair across a C 6-ring is favored. Adsorption on two hydroxyl is also clearly preferable to adsorption on one hydroxyl only (II), by 0.20 eV.

For more complex systems of functional groups in the patch on graphene used as a model of GO it is less clear which properties of the GO affect the adsorption the most. We can, however, examine whether having the chloroform H atom pointing towards or away from GO is favorable. For clean graphene it has previously been found that an orientation with H pointing away from graphene and the Cl-Cl-Cl tripod pointing towards graphene is most favorable, among the orientations considered, such as the Cl-Cl-H tripod pointing towards graphene, or the H atom pointing towards graphene. Because of the more uneven structure of the GO surface, compared to clean graphene with very little corrugation,
we cannot distinguish the orientation with the chloroform H atom pointing to GO and the Cl atoms all pointing away to the orientation with the Cl-Cl-H tripod pointing to GO, we will therefore here only distinguish the situation of chloroform H pointing mainly away from GO (“H up”) from H pointing mainly towards GO (“H down”).

Systems VIII and IX differ in principle only by the orientation of chloroform (besides the thus induced positional relaxations of both the GO and the chloroform atoms). The adsorption energies of these systems indicate that “H down” is preferable. However, results for the more complex systems X, XI and XII clearly show that there the “H up” orientation is more favorable, at least if there are functional groups on both sides of the graphene plane, but also that it matters how the Cl atoms are positioned relative to the atoms in epoxide.

Systems XIV, XV and XVI all have the same number of functional groups, placed either on one or both sides of the graphene plane. Again, the data show that placing functional groups on both sides of the plane is preferable, even when the number of functional groups are restricted and the number of functional groups close to chloroform thus becomes less, compared to having all groups on the same side as the chloroform.

The measure $h$ in Table III is an indication of the distance of chloroform from GO. Since GO is not flat, this measure is may be both shorter or longer than for example the smallest atom-to-atom distance in chloroform to GO. The $h$ measures the distance between the chloroform C atom and the closest GO O-atom, projected onto the direction perpendicular to the underlying graphene net. The values of $h$ in our calculations fall in the range 2.1 to 3.8 Å. These are reasonable distances for physisorption.

The adsorption of chloroform on clean graphene, without functional groups, was previously obtained as 0.36 eV using a similar method. This value corresponds well to the most favorable configurations for chloroform on GO systems studied here.

The information we obtain from studies like this of the physisorption of small molecules, like the binding energies and the orientation of chloroform in this study, may be useful both as direct results, but also as input for modelling of larger systems.

### C. Accuracy

We carefully check the convergence of parameters used in our QE calculations. The parameter values are changed, one by one, to slightly better and slightly worse values, and the binding energy for one of the structures with chloroform on GO is calculated. In Figure 5 we report the binding-energy dependence on unit cell size, wavefunction and density cut-off energies, the force convergence threshold value, the number of $\mathbf{k}$-points, and the vacuum size. The system studied is system II in Figure 4. The corresponding parameters are represented as a series of calculations, in which the accuracy increases going from left to right in the figure. The parameter values chosen from this convergence test for production runs are more accurate than the default values of QE. The convergence tests show that further improvements of the parameters result in changes of adsorption energies of a few meV or less.

Our calculations are carried out without correction for the dipole-dipole interaction between two copies of the system in the $z$-direction. The effect of a dipole correction on the systems is tested by applying a dipole correction along the $z$-axis, for a couple of our systems, in a manner described in Refs. 48 and 49. An example of a dipole correction test is presented in Figure 6. The electrostatic potential (ESP) curves with and without dipole correction are almost overlapping in the figures, and hence, for clarity 100× the difference of these two curves is also plotted. We see that the dipole correction only has minor effects on the (binding) energy values of the studied systems. This is not a trivial result, because the GO slab and chloroform are both polar objects. However, the difference in binding energies with and without an applied dipole correction is only 0.5–1.0 meV in most of the studied systems, with one exception showing a less than 10 meV difference.

### IV. CONCLUSIONS

We present a computational study of chloroform physisorption on GO using DFT calculations with the vdW-DF-cx method. The binding energy values vary from approximately 0.20 to 0.40 eV, depending on the local

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**TABLE III. Binding energies $E_b$ of chloroform on GO and height $h$ of chloroform above a GO O-atom (see Figure 4 for the GO-chloroform system numbers). GO# refers to the GO structures of Figure 3 and Table I.**

| System | CCl$_3$H orient. | GO struct. | GO# | $E_b$ [meV] | $h$ [Å] |
|--------|------------------|------------|-----|------------|--------|
| I      | H up             | O          | GO1 | 257        | 3.34   |
| II     | H up             | OH         | GO2 | 181        | 3.45   |
| III    | H up             | 2O         | GO3 | 225        | 3.56   |
| IV     | H up             | 2O         | GO4 | 382        | 2.72   |
| V      | H up             | 2O         | -   | 268        | 3.40   |
| VI     | H up             | 2OH        | -   | 390        | 2.14   |
| VII    | H up             | 2OH        | GO6 | 199        | 3.69   |
| VIII   | H up             | 2O, OH     | GO7 | 219        | 3.81   |
| IX     | H down           | 2O, OH     | GO7 | 286        | 3.12   |
| X      | H down           | O, 2OH     | -   | 319        | 2.99   |
| XI     | H down           | O, 2OH     | -   | 296        | 2.99   |
| XII    | H up             | O, 2OH     | -   | 422        | 2.44   |
| XIII   | H up             | 2O, 2OH    | -   | 243        | 3.45   |
| XIV    | H up             | 3O, 2OH    | GO9 | 275        | 3.79   |
| XV     | H up             | 3O, 2OH    | GO10| 333        | 2.88   |
| XVI    | H up             | 3O, 2OH    | -   | 391        | 2.59   |
FIG. 4. Adsorption of chloroform on GO. Shown are top and side views of optimized geometries in systems I–XVI, obtained with the method vdW-DF-cx. Only a part of the unit cell is shown. The corresponding binding energies are presented in Table III. Color legend for atoms: green Cl; yellow C; red O; blue H.

FIG. 5. Convergence tests of calculations for chloroform on GO. For these tests the chloroform-GO system described as number II of Figure 4 is used. In this test all calculations use the same parameter values as the production runs (“Test setup 0”) except for one parameter, the parameter indicated in the key of the figure. Lines are for ease of identification.

Further, we document the ability of vdW-DF-cx of balancing the sp\(^2\) and sp\(^3\) bindings of the GO C atoms. We do this by comparing the formation energy of the unsaturated GO structures, going from pure sp\(^2\) binding in clean graphene to a mixture of sp\(^2\) and sp\(^3\) in the formation of GO from graphene. The GO structures are structurally relaxed with use of either the semilocal PBE or the vdW-DF-cx functionals. Besides a small offset in the formation energies common to all the structures, we find the same formation energies for PBE and vdW-DF-cx calculations, underlining the ability of vdW-DF-cx of handling the change from sp\(^2\) to sp\(^3\) bindings.

Our results for chloroform adsorption may be used as input data for modelling larger systems, with or without thermodynamics, with or without additional molecules, such as water or ions. While our study is not exhaustive in searching for all possible physisorption geometries we have included a number of structures such that we have covered many of the relevant local environments of GO functional groups.

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FIG. 6. Effect of the dipole correction on the electrostatic potential in GO-chloroform systems. The plot shows a potential line scan along the box $z$-axis through the chloroform C atom (perpendicular to graphene) for the systems (a) II and (b) IV shown in Figure 4. To illustrate the length scales and positions of the constituents a piece of the GO slab and (b) IV shown in Figure 4. The plot shows a potential line scan along the box $z$-axis through the chloroform C atom (perpendicular to graphene) for the systems (a) II and (b) IV shown in Figure 4. To illustrate the length scales and positions of the constituents a piece of the GO slab and (b) IV shown in Figure 4. The plot shows a potential line scan through the chloroform C atom (perpendicular to graphene) for the systems (a) II and (b) IV shown in Figure 4. To illustrate the length scales and positions of the constituents a piece of the GO slab.
Open-source, grid-based PAW-method DFT code GPAW, http://wiki.fysik.dtu.dk/gpaw/

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