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Interaction of C_{60} molecules on Si (100)

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Abstract

The interactions between pairs of C_{60} molecules adsorbed upon the Si (100) surface have been studied via a series of DFT calculations. Configurations which have the fullerene cage located within the dimer trench bonded to four dimers (t4) have been investigated, as these have previously been found to be among the most stable for the C_{60} molecule. These t4 configurations are explored with all possible pairs of fullerene configuration combinations considered. We have looked at two distinct groups of separation distances between the two C_{60} molecules. These have the fullerene bonding sites as either adjacent to one another or separated by one Si surface dimer. Comparisons between the two groups confirm the trend of the combinations becoming more favourable at a greater fullerene separation. In the systems with adjacent bonding sites the combined pair of fullerenes were in general less favourable than the two isolated cases. At the longer fullerene separation distance this trend was reversed. The longer fullerene separation distance reflects the experimental separation observed by Moriarty *et al.* [1].

Key words: Computer simulations, Density functional calculations, Chemisorption, Silicon, Fullerenes
PACS: 61.46+w, 61.48+c, 71.15Mb

1 Introduction

The fullerene allotrope of carbon was discovered over twenty years ago. To describe the structure for this super stable cluster of 60 carbon atoms (for it was the C_{60} molecule that was the first observed fullerene) a truncated icosahedron was suggested. This structure consists of 20 hexagonal faces and 12 pentagonal faces. The C_{60} molecule was named buckminsterfullerene, after Richard Buckminster Fuller, a world renowned architect whose famous geodesic dome

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structures demonstrated a startling similarity to the newly discovered carbon molecule. The discovery of the fullerene molecules led to Kroto, Curl and Smalley being awarded the Nobel Prize for Chemistry in 1996.

The C_{60} fullerene has been successfully manipulated across a Si surface with a scanning tunneling microscope (STM) tip [2,1,3]. During manipulation only a small amount of the surface of the fullerene molecule actually interacts with the Si substrate, because of the the curvature of the fullerene molecule. Different STM tip motions have been shown to offer differing success rates for C_{60} manipulation, with both a sweeping motion [2] and a repulsive mechanism [3] explored. The STM tip used has been shown to have an impact on the success rate of the manipulation [2]. It has been proposed [3] that during the manipulation on the Si (100) surface, the C_{60} molecule rolls across the surface forming intermediate metastable adsorption configurations with the surface in order to pivot over. This results in the breaking of C-Si bonds which controls the motion of the C_{60} molecule, leading to a complex sequence of coupled rotational and translational dynamics.

The separation distances for pairs of C_{60} molecules upon the Si (100) surface have been explored experimentally [1]. When attempting to manipulate one C_{60} molecule towards a second C_{60} molecule, again via STM tip manipulation, the closest the fullerenes could be moved together was $\sim$ 10.9 Å. The only way the two fullerenes would sit that close was for one of the fullerenes to "hop" over into an adjacent trench. The closest the two fullerenes could be manipulated to one another, and have both molecules remain within the same trench, was $\sim$ 11.5 Å.

A number of differing solid-state quantum computing architectures have been proposed that rely on the unique properties of endohedral fullerenes, primarily the spin properties of the endohedral atom and the Faraday cage like properties of the fullerene molecule, in order to represent the quantum bits (qubits), within the system. Some of these schemes suggest the usage of chains of endohedral fullerenes, with alternating endohedral species (nitrogen and phosphorus are discussed as candidates) [4,5]. The use of both the electronic and nuclear spin as qubits has also been discussed [5]. We explored the suitability of N@C_{60} molcules in our previous study [6], and concluded that they met the required criteria for use as qubits. There are still some fundamental issues that need to be addressed with an architecture of this type, for example the qubit readout, however various solutions have been suggested [5].

The adsorption of fullerene molecules onto the Si (100) surface has been extensively studied with density functional theory (DFT), including the study of C_{60} molecules [7–10], C_{82} molecules [11] and capped nanotubes [12]. The studies of C_{60} molecules on Si (100) have found four groups of configurations for the C_{60} molecule upon the silicon surface. These are above the dimer trench, bonded

to either two or four dimers (denoted as t2 and t4 respectively), and above the dimer row, bonded to either one or two dimers (denoted as r1 and r2 respectively). Many studies [13–19] have been carried out experimentally which show that the C_{60} molecule adsorbs in the dimer trench at room temperature, and is only observed above the dimer row when the system is heated.

Here we examine pairs of C_{60} molecules, orientated in the t4 group of configurations (which is arguably the most stable of the four configuration groups), upon the Si (100) surface, with a view to exploring the separations between the fullerenes observed experimentally [1]. To this end we have studied the seven orientations of the C_{60} molecule that are symmetrically viable and have been found to be stable [7–11]. Furthermore, we have looked at two groupings of separation distances, one shorter than seen experimentally, and one around the experimental distance (within the same trench). The shorter separation distance, which corresponds to the fullerenes bonding on adjacent sets of Si surface dimers, has been studied in order to understand why the aforementioned fullerene "hop" occurs for fullerenes at this separation distance. The longer separation distance, which corresponds to the two fullerene bonding sites being separated one the surface by a single set of Si surface dimers, has been explored in order to understand how the orientations of the two C_{60} molecules can affect the energetics of the system.

2 Methodology

For all of the calculations presented here we have employed the density functional theory [20,21] package PLATO [22], which utilises a localised orbital basis set. The Perdew-Burke-Ernzerhof GGA [23] has been used for the exchange-correlation potential, as the LDA has been shown to overbind for systems such as the one studied here. Pseudopotentials of the type described in [24] were used to model the electron-ion interactions. Periodic boundary conditions have been imposed in all directions, and due to the size of the system, all the calculations have been carried out using just the Γ-point for k-point sampling.

The Si (100) surface has been represented by a 384 atom supercell, which is illustrated in Figure 1. This supercell was been designed in order to reduce the interactions between the fullerene molecule(s) and the periodic repeats. To this effect the size of the surface has been considerably increased from the previous computational studies of isolated C_{60} molecules [7–11], and the surface has been designed so that the surface has non-orthogonal cell vectors and the dimer rows do not run perpendicular, or at 45°, to the cell vectors; which means that the supercells main dimer row conects to another dimer row of the periodic repeat.

With the exception of these changes, the other characteristics of the Si (100) surfaces implemented in previous studies [7–11] are inherited here. Thus our model consists of six layers of Si atoms, with the bottom two layers of Si atoms being pinned in their respective bulk; and the bottom layer's dangling bonds are saturated with H atoms (which in turn have been pinned in their own relaxed positions). As with our previous study [6], we have chosen a 2 × 2 tilted dimer reconstruction, as this has been shown to be energetically most favourable within our approach [9]. A large vacuum gap has been included above the Si surface; this vacuum gap ensures a sufficient distance between the top of the fullerene cage(s) and the bottom of the surface for the periodic repeat, so as to minimise the interaction between the two.

The differing atom species present in the simulation cell are described by a series of basis sets that vary greatly in complexity (the same basis sets as used in our previous study [6]). The simplest description is for the H atoms, is described with a single s function; as the only purpose of the H atoms in our simulation cell is to saturate the dangling bonds from the final Si layer, so a more complete description is not necessary. The Si and C basis sets consist of three sets of s, three sets of p and two sets of d functions, which accounts for 22 basis functions per C and Si atom. Basis sets of this level of completeness have been shown [11] to reduce the basis set superposition error (BSSE), without the need to correct the results via the the Boys and Bernardi counterpoise method [25].

The commonly used measure of assessing the favourability of a specific orientation of an isolated fullerene cage on the Si surface, is the binding energy between the fullerene cage and the Si surface, which is the calculated as the difference between the sum of the energies of the relaxed components and the energy of the relaxed combined system (see Equation 1).

$$E_{\text{binding}} = E_{\text{fullerene on surface}} - E_{\text{isolated fullerene}} - E_{\text{isolated surface}} \tag{1}$$

As with the isolated fullerene case, one way in which to assess the favourability of the combined pairs of fullerene molecules is the calculation of the binding energy for the combined system, which is given in Equation 2. This is shown for two configurations, A and B, and in the subsequent calculations these were replaced with combinations of configurations.

$$E_{\text{binding of A-B}} = E_{\text{A-B}} - 2 \times E_{\text{isolated fullerene}} - E_{\text{isolated MF surface}} \tag{2}$$

In order to calculate the favourability of the combined system we used the formula as shown in Equation 3; this measures the binding energy of the combined system against the binding energies of the two isolated systems. This

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provides a clear insight into the improvement of the combined system versus its isolated components, however it does not allow for direct comparison between different combined systems. This is because the measure of favourability as defined in Equation 3, only gives a measure of favourability for the specific combined and isolated systems.

$$E_{\text{favourability of A-B}} = E_{\text{binding of A-B}} - E_{\text{binding of A}} - E_{\text{binding of B}} \tag{3}$$

By the way that the favourability measure is defined, a positive energy indicates that the combination of configurations is less favourable than the two fullerenes in isolation. A negative energy therefore indicates that the combination of configurations is more favourable than the two fullerenes in isolation. The separation distance between the two fullerene cages is measured as the distance between the centre of mass of each fullerene cage.

When placing two C_{60} molecules upon the Si (100) surface there are a vast array of possible arrangements and configurations. For this study we chose to focus on seven configurations from the t4 configuration group that are illustrated in Figure 2. Even when the possible configurations are narrowed down to these seven, there is still a lot of variation in the possible arrangements. Since the two fullerenes are in close proximity, the interaction between the two molecules will be most significant in the regions of the two cages that are closest to one another. When considering this, we included 180° rotations of each configuration, this further complication also affected which regions of the two fullerene cages interacted with one another. The symmetry of the t4 fullerene configurations has been employed in order to ascertain a set of unique fullerene pairing combinations.

The t4a, t4d and t4i configurations possess a plane of reflective symmetry through the centre of their bonding site. This is illustrated in Figure 3 for the case of the t4a configuration. All of the configurations were analysed individually in the manner presented in Figure 3, and the interactions with each of the other configurations was considered in-depth. In these cases the plane of reflective symmetry reduces the number of unique combinations these configurations can produce. The t4h configuration has been treated as having a 180° rotational symmetry, but no planes of reflective symmetry (due to the configurations unique "rotated" positioning). The t4h configuration does posses an equivalent rotational configuration, in which the fullerene molecule is rotated by 60°, however we have chosen not to include this equivalent configuration as it would further complicate the proceedings.

We treated two of the t4 configurations as possessing both 180° rotational symmetry and two planes of reflective symmetry, the t4b and t4c configurations. As can be seen in Figure 2 there is no issue with assuming this level of

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symmetry for the t4c configuration, however, the t4b configuration is a little more problematic. It was felt that the arrangement of the C atoms in the fullerene cage that form the C-Si binds would only lead to a small "slide" of the C_{60} molecule perpendicular to the direction of the trench, which we felt was not significant enough to warrant different treatment. The remaining configuration, the t4g configuration, is unique amongst our chosen t4 configurations in that it possesses no symmetry, which is clear when studying Figure 2. These set of carefully considered assumptions result in a set of 54 distinct fullerene pairing combinations.

The 2×2 surface reconstruction has been used in all of our calculations presented here, which due to the alternating nature of the Si surface dimers creates a problem. Within our study we have investigated what happens when one of the two C_{60} molecules rolled closer to the other. We have chosen to look at this by looking at two sets of distinct separation distances. These two sets result from having two general separation distances between the fullerenes, the first having the pair of fullerenes sitting on adjacent bonding sites (the shorter separation distance) and the second having the pair of fullerenes on bonding sites that are separated by one Si surface dimer (the longer separation distance). For the shorter separation distance the two fullerene bonding sites are identical in terms of the orientation of the surface Si dimers. This is, however, not the case for the longer separation distance, as the alternating nature of the 2×2 surface reconstruction leads to a difference in the two bonding sites. After careful consideration it was decided to treat the two bonding sites at both of these separation distances as being equivalent; again the decision came down to a question of the potential value in treating the two sites as unique, compared to the inevitable computational cost.

In order to ascertain the favourability of pairs of C_{60} configurations, first the calculation of the binding energy of a single C_{60} molecule upon the Si (100) surface in all of the chosen t4 configurations is required. The binding energies of these systems are presented in Table 1, alongside the corresponding energies from our previous study [6]; the previous study used a smaller 128 atom Si (100) surface which has been used extensively in other studies [7–11]. As Table 1 illustrates, there appears to be a shift in not only the magnitude of the binding energies, with every configuration becoming less favourable on the larger surface, but the ordering of the favourability hierarchy has also changed. For the t4d case in particular, the length of the one long C-Si bond goes from 2.73 Å, with the 128 atom surface, to 2.43 Å with the new surface. This could indicate that the increased bond length for the 128 atom surface, with the t4d configuration, is a result of the surface size.

We attribute the decrease in system favourability in all configurations to a interesting concept of note, namely, that to an extent the fullerenes actually prefer sitting in proximity to one another. The previous smaller surface con-

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sisted of two rows of four dimer pairs; this means that the periodic repeats of the fullerenes upon the surface only had two dimer pairs between the fullerene bonding site and its periodic repeat. In terms of separation across the trenches, there will only be one empty trench between the fullerene bonding site and its periodic repeat. With the new larger surface the distances between the periodic repeats are much greater; there is a two trench gap between periodic fullerene repeats, across the rows, and there are twenty-two Si surface dimers between the periodic fullerene repeat within the same trench. This larger surface was specifically designed to increase the distance between these two periodic repeats. In doing so, however, the non-uniform nature of the supercell leads to other periodic fullerene repeats that are, at times, closer than the intial two repeats. There is now, for example, a periodic fullerene repeat in the trench adjacent to the fullerene in the original supercell, which is separated by six Si surface dimers.

We explored the impact of the periodic fullerene repeats and found that for the repeats within the same trench and across the dimer rows, even when the repeats are separated by over 60 Å, there is still some level of interaction. The influence of the repeat within the same trench is greater, and in general as the distance is increased, in both directions, the binding energies become less favourable. This indicates that to an extent fullerenes are more favourably adsorbed onto the Si surface within a close proximity of other fullerene molecules (although not at the shorter distances explored later on in this study).

In terms of the calculations performed with the smaller surface [7–11] and our own study [6], it would appear that there is a level of interaction with the periodic fullerene repeats. This has almost certainly made the binding energies more favourable, however, while not ideal, the simulation cell is more than adequate. With the larger 384 atom Si surface the interaction from the two types of repeats studied here is less of an issue, certainly the periodic fullerene repeat within the same trench. The problem with this surface is its non-uniform nature which leads to other periodic repeats, as the level of influence of these are much harder to gauge. Until either the computational effort is reduced, or the computational resources available increases, this will remain a topic of which further study could be performed. Although, as always the effort in doing so has to be weighed against the possible gain and its actual worth.

3   Results

For the fullerene pairings whose fullerene bonding sites were separated by one Si surface dimer the full set of 54 unique combinations of fullerene configurations have been successfully modelled and the measures of favourability and

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separation have been calculated. The fullerene pairings with adjacent bonding sites were not as fruitful, with only 49 out of the 54 unique combinations being successfully modelled, of which only about half of the calculations relaxed into the desired configurations. This can be attributed to the proximity of the fullerene cages, as often the cage with the weaker bonds would reorientate itself, often resulting in less C-Si bonds being formed and less favourable energies. This is not an issue with the longer fullerene separation distance, and in all cases all C-Si bonds are formed (four per C_{60} molecule). Another marked difference between the two separation distances, which again is a direct result of the differences in fullerene separation, is that in the longer separation fullerene systems there is no evidence of any C-C bonding taking place between the two C_{60} molecules; the shorter separation systems have a handful of combinations that possess significant and complex C-C bonding occuring between the two fullerene cages.

For both of the two general separation groups, the range of the separation distances, between the two C_{60} molecules, for the all the combinations we have studied is ~ 1.5 Å. For the longer separation systems this range is slightly more than we expected to see, as with the shorter separation, some of the combinations experienced bonding between the two fullerenes which would significantly reduce the distance between the two cages. For the longer separation fullerene systems, the majority of results, in terms of the separation between the two fullerene cages, seem to be centred around the separation distance of 11.5 Å, which corresponds to the distance found in the experimental study [1] when the two fullerenes were in the same trench. This is less clear cut with the shorter separation fullerene systems, with a reasonable amount of the results falling between ~ 9 to 9.5 Å, and the remaining ones spread between ~ 8 to 9 Å.

In terms of system favourability for the longer separation systems, the vast majority ($\sim 94\%$) of the fullerene combinations are more favourable when considered as a combination pair, rather than as individual configurations. This is markedly different for the shorter separation systems with only one of the fullerene combinations being marginally more favourable as a pair than in its isolated components. The remaining fullerene combinations are all less favourable as a pair, in some cases this is by a substantial amount (~ 6 to 14 ev). The range of favourability for the longer separation systems is ~ 1 eV, which is significantly smaller than the range in favourability found in the shorter separation systems of ~ 14 eV. We attribute this to two factors, firstly the bonding between the fullerenes for the shorter separation systems have a strong influence on the binding energy. Secondly at the longer separation the orientation of the two C_{60} molecules has less influence on the binding energies.

When the results from both separation groups are combined, as shown in Figure 4, a few observations can be made. Firstly the variety within the longer

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separation systems, in terms of the favourabilities, does not seem to be sig-nifcant, especially in comparison to the variation found within the shorter separation systems. There is a trend illustrated by both sets of results, of the fullerene pairings becoming more favourable as the separation of the two fullerenes is increased. This trend is much more clearly demonstrated in the shorter separation systems. There does appear to be a general curve that could be used to represent the relationship between the separation of the two fullerene cages and the favourability of the combined system (with respect to the isolated systems). The fact that the range of separations shown for both groups are very similar demonstrates that the range of separations might have more to do with the configurations in which the two fullerenes are placed, rather than any interaction between the two cages.

It is clear from Figure 4 that the shorter separation systems are significantly less favourable than the longer separation systems, and that the separation distance between the two fullerenes is fundamental in this. The shorter sepa-ration systems often suffered from interaction between the two fullerene cages (and in some cases covalent C-C bonding between the two cages). The re-pulsive nature of the interactions between the two C_{60} molecules also caused the fullerenes in the shorter separations systems to often "roll back" away from each other, which in turn weakened the C-Si bonds. In contrast, the longer separation systems have enough of a gap between the two C_{60} cages that any interactions between the two actually have a positive impact, with the fullerenes often finding more favourable bonding conditions than their isolated counterparts.

As discussed above, the group of shorter separation systems found a few con-figuration combinations where strong covalent C-C bonding had occured be-tween the two fullerene cages; with on occasion up to six new C-C bonds being formed between the two molecules. In two of these cases the interac-tion between the two fullerenes was significant enough to greatly distort the fullerene cages involved. In these cases some of the atoms lost their origi-nal nearest neighbours and gained new ones; the resulting structures often tended to form hexagonal and pentagonal rings, although these were often distorted. As previously stated, none of the configuration combinations from the longer separation systems showed evidence of C-C bonding between the two fullerenes, which is unsurprising considering the increase in the separation between the two fullerenes.

The energies for the shorter separation systems demonstrate why fullerenes are not observed experimentally upon adjacent Si surface dimers, as these systems are very energetically unfavourable. In the calculations at the shorter distance many of the fullerenes were unable to sit in the correct positions, re-sulting in the C-Si bonds being strained (and not formed in all cases). Further more, in order to recreate certain combinations several of the systems began

with interpenetrating fullerenes, which is likely to have affected the resulting structure. Experimentally [1], when two fullerenes are tried to be manipulated into this close of a proximity, one of the fullerenes is shown to hop over to the adjacent trench, demonstrating that the two fullerene molecules do not want to come that close together. The remainder of this results section shall focus on the results of group of systems with the longer fullerene separation, as these more realistically recreate the distances observed experimentally [1] .

When comparing the average binding energy for each configuration (calculated by taking the mean value for each configuration, taking into account every combination that each configuration takes part in) with the isolated cases, the difference between all the configurations is reduced; this is unsurprising as it could be expected that some of the more favourable configurations would compensate for some of the less favourable configurations. The most significant change between the binding energies of the isolated cases and the averages of the fullerene combinations, is for the t4h configuration. One possible explanation for this improvement in the t4h configuration could be that its unique "rotated" placement on the surface, makes one region of the cage closer than the other region, to the other fullerene. In the other configurations this is a lot more uniform, so it could account for the improvement observed in the t4h configuration.

When studying the average favourability of each configuration, the improvement in the t4h configuration when it is placed alongside another fullerene, compared with when it is in isolation is further demonstrated; the t4h configuration is clearly the most favourable configuration for the other fullerenes to be combined with. This does however highlight that the t4h configuration is the most unfavourable configuration in isolation, so it is possible that this improvement has more to do with our method of calculating favourability than anything more significant. The results for the t4a configuration are interesting, as while it remains favourable in terms of the binding energies of both the isolated case and the fullerene pair combinations, in terms of average system favourability it is the least favourable of all the configurations. It is possible that this is related to the fact it has the largest bonding configuration, in terms of the area of the fullerene cage that bonds with the fullerene surface. This could lead to a greater deformation within the fullerene cage, which would affect the area of the fullerene cage that is closest to the second fullerene. The only combinations that possess a non-negative favourability (meaning that the isolated components are more favourable than the combined pair), all involve the t4a configuration, which is obviously also going to affect the average favourabilities.

As previously mentioned, three of the configuration combinations were less favourable than their isolated components. In all of these configurations the C-Si bonds formed between the fullerene molecule and the Si surface became,

in general, longer and weaker when compared to the C-Si bonds in the isolated components. The general trend for the configuration combinations was for the C-Si bonds to become shorter, stronger and more uniform (the C-Si bonds in configurations that previously had great variety in bond energy and length became similar). The t4d configurations are interesting because, as with previous studies [8,6], there is always one C-Si bond that is considerably longer than the other three. In the isolated case this C-Si bond is 2.43 Å long, but throughout the combinations explored here this bond ranges from 2.26 to 2.55 Å.

4 Conclusions

Experimentally when manipulating one C_{60} molecule across the Si (100) surface towards another C_{60} molecule,it has been shown that when the separation between the two molecules becomes less than $\sim$ 11.5 Å, one of the fullerene molecules will "hop" into the adjacent trench [1]. We have explored this situation using computational simulations to study two distinct groups of fullerene separations. The first grouping examined what would happen if the two fullerenes were adsorbed upon the Si (100) surface at a shorter distance than seen experimentally. The results for this group suggests that the reason for the experimental "hop" is because the system becomes very energetically unfavourable at this separation, causing a disruption of the C-Si bonding (a weakening of the C-Si bonds compared to the isolated cases), and in some cases a disruption of the internal C-C bonding within each fullerene molecule (due to covalent bonding occuring between the two molecules). These results indicate that the possibility of placing C_{60} molecules at such separations experimentally is extremely unlikely.

The second grouping examines a more realistic separation between the two fullerene molecules. It is clear at this separation distance (all cases were between $\sim$ 10.75 to $\sim$ 12.25 Å), which represents a one Si surface dimer gap between the fullerene molecules, that the energetics of the systems are more favourable. In fact the vast majority of cases were more favourable as a pair than in their isolated components (the complete reverse of the shorter separation distance). The general trend is for the C-Si bonds to become either shorter and stronger, or become more uniform (in the configurations with vary varied bond lengths/strengths), both of which make the bonding with the surface more energetically favourable. At this separation distance no C-C covalent bonding was observed. The second group shows an excellent agreement with the minimum separation (with both fullerenes in the same trench) found experimentally [1].

5 Acknowledgements

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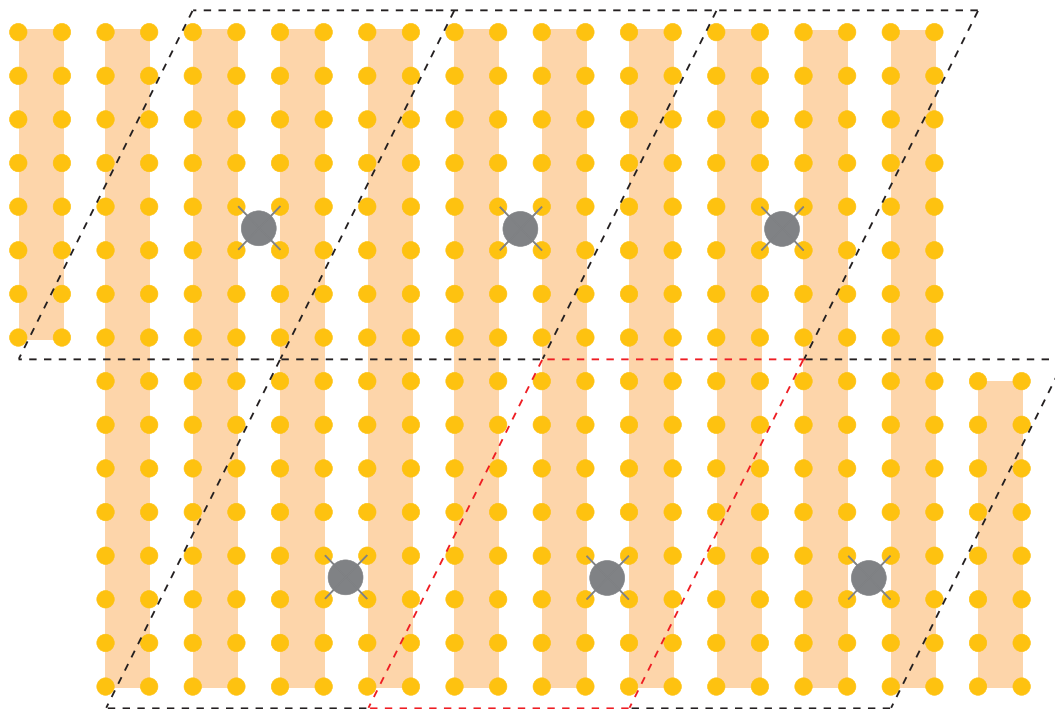[25] S. Boys and F. Bernardi, Molecular Physics 19 (1970) 553.

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Fig. 1. Top down schematic, showing only the top layer of atoms, of the 384 atom supercell for the Si (100) surface. The original supercell is the area within the red dotted line, which is shown amongst five periodic repeats, which are shown as within the black dotted lines. The fullerene in the t4 position is shown as a grey circle, the dimer rows are the pale orange bars, and the white gap between the rows represents the trench. The Si atoms that make up the surface dimers are shown as yellow circles.

Config.	Previous study [6] (128 atoms)	This study (384 atoms)
t4a	-2.84	-2.29
t4b	-3.14	-2.62
t4c	-3.14	-2.30
t4d	-2.40	-1.62
t4g	-2.77	-1.95
t4h	-2.52	-1.57
t4i	-2.41	-1.64

Table 1
Binding energies, in eV, of the C_{60} molecule, in the t4 group of configurations, for our earlier study and the results from this study.
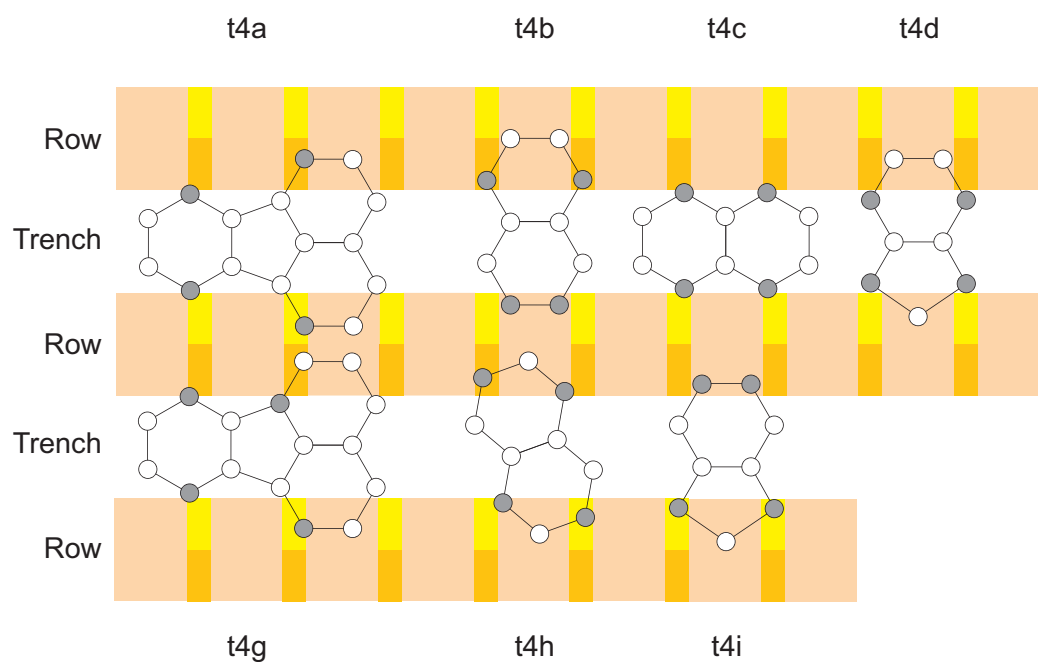
Fig. 2. Pictured above are all the t4 configurations that have been investigated in this study. The pale orange strips represent the dimer rows. The Si dimers with which the cage bonds are represented by the yellow and orange bars. The yellow part represents one Si atom of the pair, and orange part represents the other Si atom. The white region between the dimer rows represents the trench. C atoms are depicted as white circles, with the exception of those which bond with the Si surface which are depicted as grey circles.
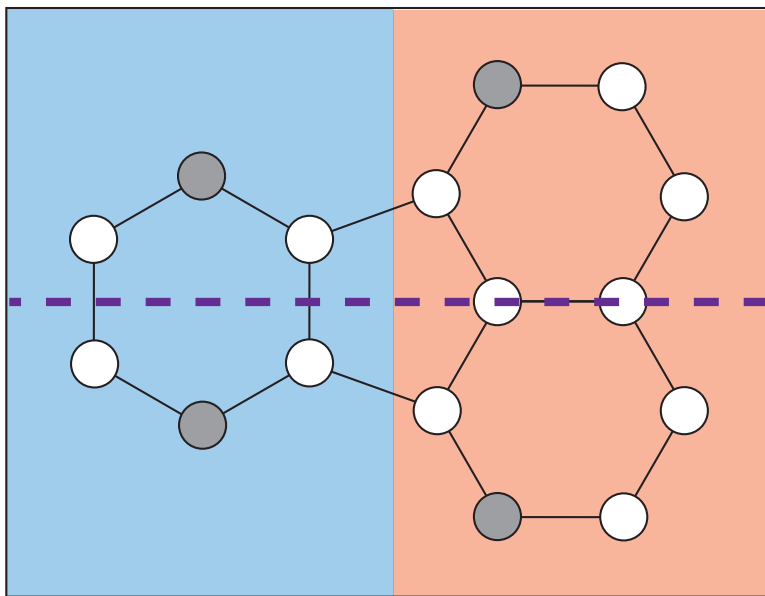
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Fig. 3. Schematic illustration demonstrating the symmetry associated with the t4a configuration. The purple dashed line represents the plane of reflective symmetry that the configuration possesses. The red and blue shading illustrates the equivalent regions within the configuration, where the two red regions (separated by the plane of symmetry) are equivalent, and likewise the two blue regions.

Fig. 4. The separation between the centres of mass of the C_{60} cages plotted against the measure of favourability for the binding energy of the combined system when compared to the isolated cases. The data is split into two groups which represent the two different groups of calculations performed. The red squares represent the shorter separation distance systems, and the blue diamonds represent the longer separation distance systems.