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Adsorption of C_{82} on Si (100)

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Abstract

The interactions between C_{82} molecules and the Si (100) surface have been explored via ab-initio total energy calculations. Configurations which have the cage located within the dimer trench bonded to four dimers (t4) and upon the dimer row bonded to two dimers (r2) have been investigated, as these were found to be most stable for the C_{60} molecule. It is found that the interactions between the surface and the C_{82} molecule are weaker than for the corresponding configurations for C_{60}. The C_{82} cage has a far lower symmetry than the C_{60} cage and this gives many more unique rotational orientations of C_{82} compared with C_{60}. We have thus investigated the binding energy when the local area of the C_{82} binding to the surface is the same but the cage orientation varies. We show that the binding energy can vary strongly within the configurations investigated. Bader analysis has been used to explain the relative binding energies of the different configurations.

Key words: Computer simulations, Density functional calculations, Chemisorption, Silicon, Fullerenes
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1 Introduction

The fullerene allotrope of carbon has attracted plenty of interest since it was discovered in 1985, mainly due to its unique cage structure. Many applications have been suggested that would harness this property in useful ways. It is thought that endohedrally-doped fullerenes are strong potential candidates to represent qubits within spin based solid state quantum computers. These would interact with quantum gates on the silicon surface that can read and input the necessary quantum states. The fullerenes need to be manipulated across the surface to certain regions where these gates are located. The

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fullerene cage's pseudo-spherical structure is thought to be an ideal housing for an endohedral species as a large cross sectional area is available to interact with a suitable manipulation device, whilst only a small region interacts with the surface.

The behaviour of the fullerene cages upon silicon is therefore intrinsically very important to the feasibility of such systems and has been studied both computationally [1–4] and experimentally [5–11]. Experimental studies have also examined the manipulation of the cage upon the surface by a suitable device, most often a scanning tunnelling microscope (STM) tip [12,13]. It is possible to move the molecules both parallel and perpendicular to the dimer rows upon the surface at room temperature although the success rate parallel to the rows is much higher [13]. A combination of experimental work and ab-initio studies have explored the details behind the movement of the C_{60} across the surface [10–12].

Experimental studies mainly show that the C_{60} molecule adsorbs in the dimer trench bonded to four dimers at room temperature [7,5,13] and only moves to sit on the dimer rows when heated. A study of C_{84} and the endohedral fullerene La@C_{82} [14] found that these larger molecules would also adsorb above the dimer row at room temperature and this was attributed to the larger radius of curvature. An encouraging result was that both of the larger molecules adsorbed in the same way, suggesting that the presence of the endohedral atom had little or no effect on the interaction between the cage and the surface.

The C_{60} molecule upon the Si (100) surface has been studied quite comprehensively with density functional theory (DFT). Initial studies [1,2] employed a double numeric with a single polarisation function (DNP) basis set and the local density approximation (LDA) exchange correlation functional and found that there are four groups of configurations that the molecule can take. These are within the dimer trench bonded to two or four dimers, and upon the dimer row bonded to one or two dimers. We will refer to these as the t2, t4, r1 and r2 sets of configurations respectively. The most stable configurations are those where four carbon silicon bonds form, in the t4 and r2 groups. A further study [3,4] identified additional configurations within the initial groups and estimated the basis set superposition error for each configuration using the Boys-Bernardi counterpoise method [22]. Although a very similar basis set was used, calculations were performed with the generalised gradient approximation (GGA) as well as the LDA.

Here we extend the initial work by re-examining the t4 and r2 configurations with a larger basis set to examine the effects this has upon the basis set superposition error. We confirm that the more complete basis set reduces the effects of basis set superposition error to a level comparable with the BSSE corrected results and then proceed to our investigation of the C_{82} molecule.

It is necessary to move to a larger molecule as the C_{60} is too small to contain many of the proposed endohedral species such as Lanthanum. C_{82} has over twice the internal volume of C_{60} and appears to be a suitable candidate.

2 Methodology

The interactions between the fullerene cage and silicon surface have been modelled using the ab-initio density functional theory method [15,16] with the localised orbital code PLATO [17]. Calculations were performed using either the Perwdew-Burke-Ernzehof GGA [18] or the LDA [19]. The electron-ion interactions are modelled using pseudopotentials of the type described in [20]. We employed a triply numeric basis set with a double polarisation function, this gives 22 basis functions per atom for C and Si atoms.

The simulation cell used for the C_{60} on Si is identical to that in [1,2] with the exception that we have used a 2×2 tilted dimer reconstruction. The C_{82} simulation cell is substantially larger, containing 338 atoms compared to 188 within the C_{60} simulation cell. This is mainly due to the Si (100) surface that has been extended in order to keep the larger C_{82} cages from interacting with each other due to the periodic boundary conditions. To increase the distance between periodic repeats of the C_{82} we have employed a larger surface cell with dimer rows running diagonally through it as opposed to parallel to the cell vectors as shown in Figure 1. The other features of the surface remain the same though, it is six layers thick and the bottom two layers are pinned in position with the dangling bonds saturated by hydrogen atoms.

There are nine isomers of C_{82} that obey the isolated pentagon rule (IPR) which states that the most stable isomers will be those for which the twelve constituent pentagons are not adjacent to one another [21]. Simulations predicted the third IPR isomer [21] to be the most stable, therefore this was selected for adsorption calculations.

A measure of the binding energy between the fullerene cage and the silicon surface is the difference between the sum of the energies of the relaxed isolated components and the energy of the relaxed combined system. Thus,

$$E_{\text{binding}} = E(\text{Fullerene on Si}) - (E(\text{Isolated fullerene}) + E(\text{Isolated surface})).$$

Although there is considerable benefit from the use of a localised basis set in terms of reduced computational cost there is an associated problem with calculations of this nature. The basis sets are incomplete and as the different

species are in such close geometrical proximity they will have their wavefunctions expanded to some extent by the basis functions of the other species. This leads to an artificially deep energy minima caused by the inconsistency between completeness of the basis sets for the isolated components and for the combined system. It is more concisely known as the basis set superposition error (BSSE).

It is possible to estimate the BSSE via a method developed by Boys and Bernardi [22] called the counterpoise method. The completeness of the basis sets in isolation are reconciled with the more complete basis set that results for the combined system and this has been used in a previous study [4]. Although the counterpoise method is generally accepted to give a good measure of the BSSE, it is also thought by many to overcorrect [23]. It is, however, important to note that this only corrects the BSSE with respect to the binding energy. All other quantities within the calculation remain contaminated by it.

Another way to counteract BSSE is to move to a more complete basis set. This is advantageous as it reduces the effects of BSSE throughout the calculation for all quantities. Previous studies [2,1,4] have employed doubly numeric basis sets with a single polarisation function for Si and C, i.e. two s and p functions and one d function for each atom. In this study we have used a triple numeric with double polarisation function (TNDP) basis set with which we perform our calculations. This more complete basis set incorporates three s, three p and two d functions and there is of course an increased computational cost associated with this. The H atoms that saturate the dangling bonds of the Si surface are still described with a single s function.

The ideas in Bader's atoms in molecules work [24] have been used to analyse the bonding and the charge transfer in the systems. The methodology for the analysis of the bonding works by locating critical points in the electron density of the system, these are points where the gradient of the density is zero. When these points lie between atoms that are bonded then the critical points are saddle points of the electron density. Furthermore if the Hessian matrix of the electron density, which consists of the curvatures of the electron density at the critical points is constructed, and the eigenvalues found. Then due to the nature of the point two of the three eigenvalues will be negative and these give the curvature of the bond in directions perpendicular to the bond. The ratio of these gives us a measure of the bond's characteristic, in particular it indicates how much π characteristic the bond has. For example, the single and double bonds found in ethane and ethene respectively have eigenvalue ratios of 1.00 and 1.27. These are what we can consider as perfect single and double bonds, bonds that have ratios between these two values are what we can consider as having some interaction between the p orbitals of the constituent atoms. As expected for C_{60} we see two distinct bond types with the weaker having a ratio of 1.12 and being located around the pentagons, the stronger bond type has a

ratio of 1.18 and are located at bonds shared by hexagons. The Bader analysis in this work has been performed using the algorithm devised by Sanville *et al.* [25].

The Bader charge analysis works by defining a volume around the atoms and calculating the charge contained within the volume surrounding each atom. The volumes are defined by mapping out the surface of zero flux between atoms, *i.e.* the surface where the gradient of the density in direction of the normal to the surface is zero. This allows the charge on the atoms to be calculated in a way that is independent of the basis set for a given charge density, unlike Muliken population analysis, thus leading to a more rigorous definition of the charge on an atom within the constraint that the charge on an atom in not a quantum mechanically observable quantity.

3   Results

Previous studies involving C_{60} have identified four groups of configurations that the cage can take upon the surface. In this paper we focus on the two of these that produced the most stable structures, those with the cage on the dimer row centred between two dimers (r2) and with the cage in the dimer trench bonded to four dimers (t4). These are shown in figures two and three respectively. We have replicated all of the previous structures identified in [1] and some of the additional structures from [4]. We were unable to simulate t4e, t4f and t4j; t4e relaxed into the t4g configuration and both t4f and t4j moved into the highly stable t4b configuration. It is evident from table 1 that the results gained using the TNDP basis set are in reasonable agreement with the BSSE corrected results from [4] which were obtained with the less complete basis set. The TNDP results are, however, seen to give results which are more tightly bound, which is in line with comments that the counterpoise method is thought to overcorrect [23].

The differences between the C_{60} and C_{82} cages extend much further than just a difference in the number of constituent atoms. The highly symmetric nature of the C_{60} cage is reflected in the bonding between atoms, with only two types of bond existing. Between adjacent hexagons there are what can be considered double bonds and between adjacent pentagons and hexagons we see bonds that are close to being single bonds. In reality these bonds are not perfect single and double bonds that exist in alkanes and alkenes respectively, but the point is that there are just two distinct bond types within the cage. The case for the much less uniform C_{82} cage is very different. Bond energies and orders vary much more widely and although most fall within the range of the bonds in the C_{60} case most cannot be classified as nominally single or double bonds.

Bader analysis [24] using the methodology developed by Sanville *et. al* [25] has been performed on each of the isolated cages to produce a clearer illustration of the differences between the bonding in each of the molecules. For the case of the C_{60} molecule as stated earlier we found two different bonds, the case for C_{82} though is quite different. There is a much broader spectrum of ratios of the eigenvalues, although almost all of the bonds fall between the stronger and weaker bonds in the C_{60}. The overall picture is of a much less uniform bonding structure, although there is a similarity to the C_{60} in that the pentagons tend to be surrounded by bonds that are closer to single bonds.

The less uniform structure presents us with issues with regards to placement on the surface. For the C_{60} molecule every hexagon is equivalent to every other hexagon with regards to its surroundings. The same is true of the pentagons due to the molecule being an IPR isomer. This means that any region of the cage, however large, is non-unique, the same is not true for the C_{82} molecule. Although we again consider an IPR isomer so we know that the immediate surroundings of the pentagons are unique, that is all that we can be sure of. This gives us many more options for placement upon the surface. For instance, when considering the r2 set of configurations we have seven ways of placing the C_{60} cage down in order for it to bind to 2 dimers upon the dimer row, these are shown in figure 2. Taking r2b as an example, we see that the atoms that bond to the surface are contained in a hexagon and an adjacent pentagon. Whichever pentagon and hexagon we chose to place in this position would not matter for the C_{60} as all are equivalent and have equivalent surroundings. For the C_{82} molecule we must be more precise though. If we just consider the ring of hexagons and pentagons immediately surrounding the hexagon and pentagon that contain the bonding atoms for C_{82} then we already have three options, these are shown in figure 4. As can be seen from this figure the choice of site has a large effect on the curvature of the cage in the region that is bonded to the surface, with the cage with the least amount of pentagons in the region having the smallest curvature. The number of placement options increases rapidly as we consider the arrangement of hexagons and pentagons over a larger region of the cage. For other configurations we see a similar picture. For configurations where two hexagons contain the atoms bonding to the surface (r2a, r2e, t4b, t4c) there are 6 possible ways to place the C_{82} cage down when considering only the region immediately surrounding the atoms that bond to the surface.

As there are so few regions that can be considered as equivalent, it is necessary to chose more than one orientation of the cage for each configuration that is being investigated. We have investigated a small selection of configurations and have performed three separate calculations for each by choosing different regions on the cage. Orientations of the cage were chosen by mapping the molecule and comparing local regions that would be bonding to the surface. It was decided to distinguish these regions by the amount of pentagons

within them. The pentagons are significant as they supply the curvature to the cage and bring with them an associated amount of strain energy. Figure four displays the three orientations of the cage upon the surface within the r2b configuration, each with a different number of pentagons located in the vicinity of the bonding region. Results presented here have been calculated with the TNDP basis set and within both the LDA and the GGA.

It is apparent from table 2 that the binding energies to those for C_{82} on Si (100) are in general smaller than those for C_{60} in the corresponding configuration, implying that the C_{82} molecule interacts less strongly with the surface. It is also apparent that the binding energies in some cases vary widely depending on the surrounding topology. It is also, however, evident that the effect is not consistent, for instance the two orientations of the cage within the r2a configuration which are most different in terms of surrounding environments are actually very close in energy, but in configuration t4c the reverse is true. It is therefore necessary to look in more detail at what is happening to the fullerene cages upon binding to the surface.

Bader bond analysis of the combined systems has been carried out and reveals a trend between the amount of bonding rearrangement within a region of the cage and the strength of interaction. The clearest way to define this region is to think of the molecule in terms of layers. The first layer is the part of the cage that contains the carbon atoms that have bonded to the surface, depending on the configuration this is either one hexagon, one pentagon or a combination of two (due to the IPR only hexagon-hexagon or hexagon-pentagon are seen here). The next layer is the ring of hexagons and pentagons that surround the first and so on. The bonds in the second layer that effectively link the first and third layers appear to be key. When the negative eigenvalue ratios at these particular bond critical points are compared with those in the isolated cage we see a distinct trend between the strength of the interaction with the surface within a particular configuration and the change in the ratios. The stronger binding energies within each set of orientations of the cage for a certain configuration have less change in the ratios of the eigenvalues than the weaker ones. This is very much in line with the earlier findings in the work on C_{60} on Si (100) that the less bond rearrangement there is the stronger the binding energy is. This is illustrated in figure 5 for the r2b case, where the region of the C_{82} molecule around those that bind to the Si surface is shown; the atoms represented by larger circles are the ones that form Si-C bonds. The numbers next to the bonds are the ratio of the eigenvalues after the C_{82} molecule has bound to the surface with the ones in brackets being from before it binds to the surface. It can be seen that for all three cases the bonds marked a and b become notional double bonds, whereas in the region containing the bonds c, d and e considerable delocalisation can be seen. The results of this analysis for all the cases is given in table 3, it can be seen that of the twenty seven configurations examined, there are only five outlying results, the least

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well bound cases for r2e, r2f, t4b, t4c and t4g. These outliers can, however, be explained by inspecting the strength of the Si-C bonds formed, in these five cases weaker Si-C bonds are formed than is normal. In fact for two of the cases less than four Si-C bonds form; three in the case of r2f and two in the t4c case.

Bader charge analysis of the combined systems reveals more charge than was previously thought is transferred from the silicon atoms to the carbon atoms that are involved in the bonding between cage and surface. Typically between 0.3 and 0.5 electrons are transferred onto the carbon atoms. A previous study [2] used Mulliken population analysis and found a much smaller charge transfer, with at most 0.1 electrons transferred on to the carbon atoms.

4 Conclusions

The C_{60} results show us that the more complete basis set, whilst being significantly more computationally expensive does reduce the BSSE to a level comparable with other uncertainties in the calculations. Although it is possible via the a posteriori counterpoise method to achieve similar binding energies it must not be forgotten that all other quantities will still be contaminated by the effects of BSSE.

The C_{82} molecule can be placed on the surface in the same way as the C_{60} but there are many orientations within each configuration that the C_{82} cage can take. The energies vary considerably depending on the orientation of the cage. Bader bonding analysis shows us that the group of bonds lying in a certain region of the cage close to the area that binds to the surface are key to explaining this. The change in the characteristics of these bonds correlates well with the bonding energy for a given configuration. The change in the eigenvalues is measuring the rebonding that is taking place in the C_{82} thus this gives a similar picture to what was seen previously for the C_{60} molecule, what it does not give, however, is a method of comparing molecules in different configurations.

The C_{60} molecule has the strongest binding energies when placed in the dimer trench and bonded to four dimers. For the C_{82} molecule, of the configurations investigated here, we see stronger binding energies when it is placed on the dimer row bonded to two dimers. The average binding energy upon the row for C_{82} is roughly twice as high as that for within the trench. Interestingly though, both cages have the same two configurations at the top of their energy hierarchies although in different orders (t4b and r2a). This is in agreement with experimental results on this system [14] where C_{82} molecules are observed to be sited in both trench and row sites in contrast to the case for C_{60} molecules

where they are only observed in trenches, unless heated.

Bader charge analysis shows that substantially more charge is transferred to the carbon atoms from the silicon than was seen previously [2] when Muliken population analysis was used.

5   Acknowledgements

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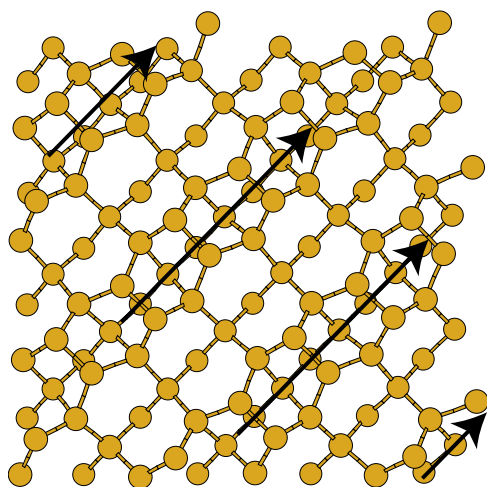[25] E. Sanville, S.D. Kenny, R. Smith and G. Henkelman, J Comput. Chem. 28 (2007) 899.

Fig. 1. The above figure displays the top two layers of atoms of the new surface used for simulations involving C_{82}. Dimer rows now run diagonally through the surface, increasing the distance between periodic repeats of the molecule in the same trench or upon the same row by approximately 40 %.
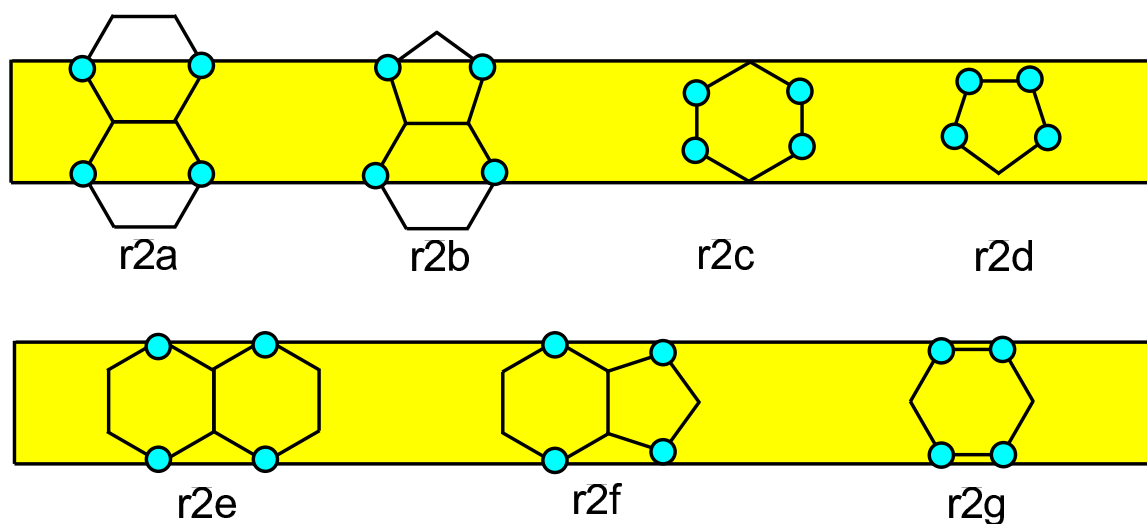
Fig. 2. Pictured above are all of the r2 configurations that have been investigated in this study. The yellow strips represent dimer rows. Carbon atoms that bond to the surface are depicted as blue circles.
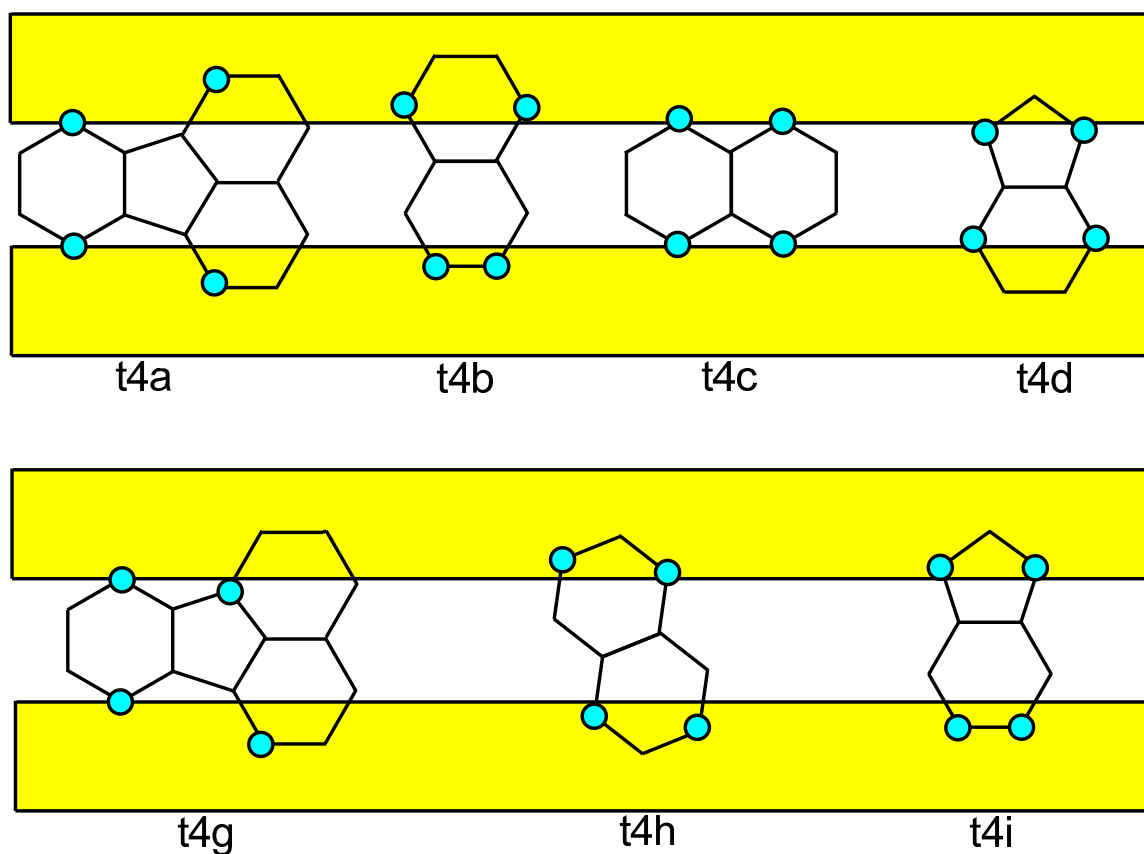

Fig. 3. Pictured above are all of the t4 configurations that have been investigated in this study. The yellow strips represent dimer rows and the spaces between them are dimer trenches. Carbon atoms that bond to the surface are depicted as blue circles.
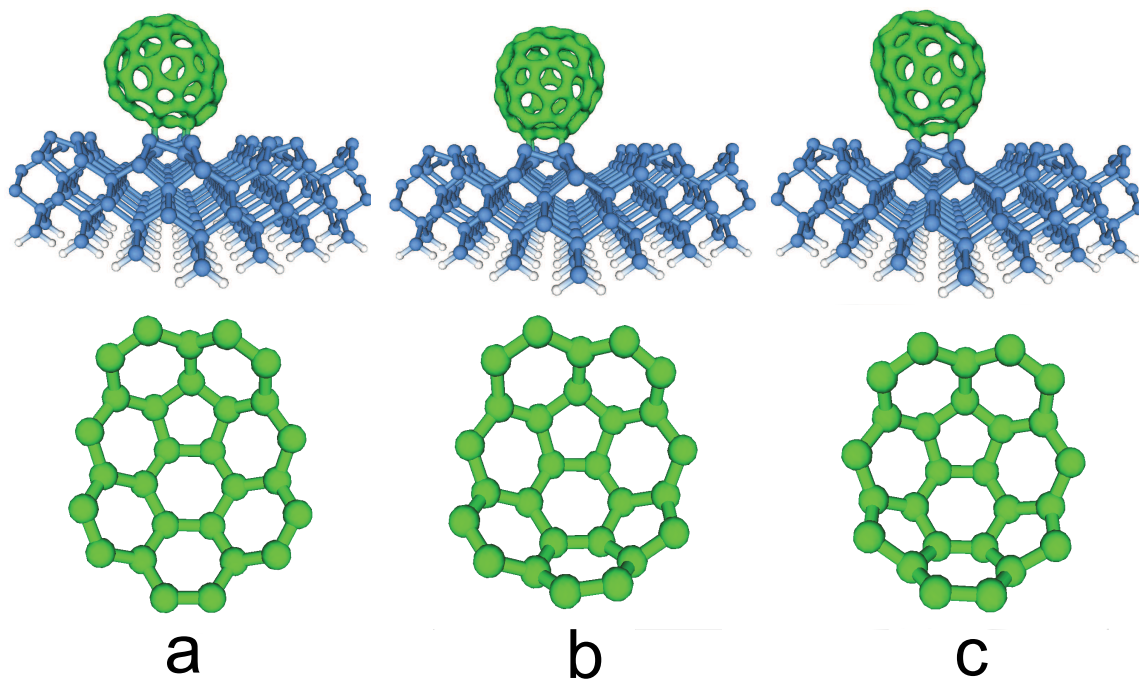
Fig. 4. Three different orientations of the C_{82} cage within the r2b configuration. The local region of the cage that bonds to the surface in each instance is shown in the lower part of the figure. Of the three different orientations, case a has no pentagons in the region surrounding the central pentagon and hexagon that contain the atoms that bond to the surface. Case b and c have 1 and 2 pentagons in this region respectively and their effect on the curvature in this region can be seen clearly.
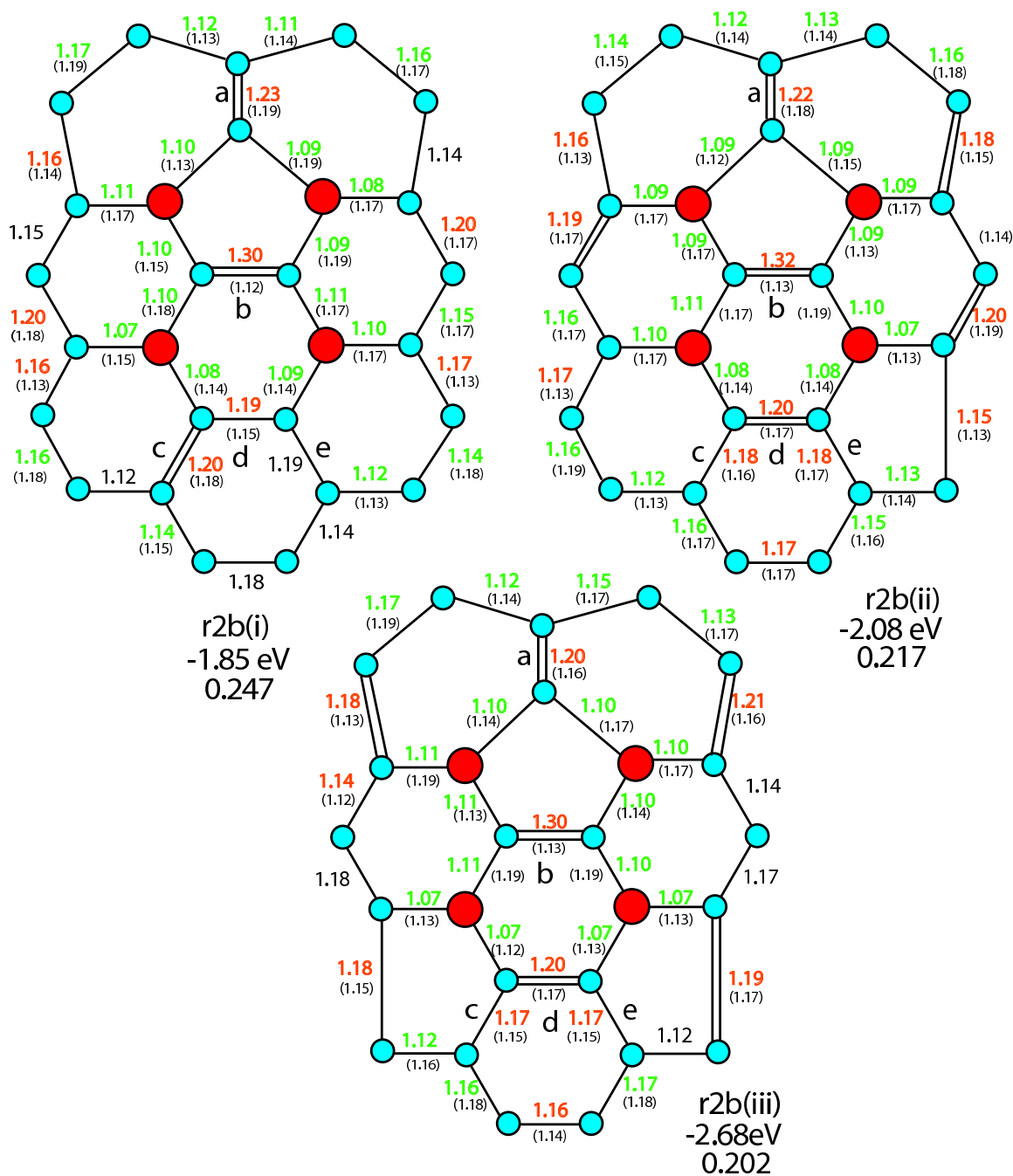
Fig. 5. Bader bonding analysis of the C_{82} molecule in the three r2b configurations. The local region of the cage that bonds to the surface in each instance is shown in the figure, the atoms represented by the larger circles are those that bind to the Si surface. The numbers give the ratio of the negative eigenvalues at the bond critical points in the Bader analysis with the numbers in brackets being the values for the isolated fullerene.

Configuration	SIESTA DZP[4]	PLATO TNDP
t4a	-2.16	-2.77
t4b	-2.53	-3.15
t4c	-2.63	-3.02
t4d	-1.96	-2.32
t4g	-2.53	-2.78
t4h	-1.94	-2.35
t4i	-1.83	-2.45
r2a	-2.58	-3.02
r2b	-2.49	-2.72
r2c	-2.00	-2.82
r2d	-0.87	-1.29
r2e	-1.69	-2.16
r2f	-2.19	-2.32
r2g	-1.10	-1.42

Table 1
Binding energy results using the GGA for C_{60} on the Si (100) surface in electron volts. The results from [4] have had the BSSE estimated and removed via the counterpoise method. For more information regarding the details of each individual configuration see [2,4].

	Orientation 1		Orientation 2		Orientation 3	
Configuration	LDA	GGA	LDA	GGA	LDA	GGA
r2a	-3.60	-2.39	-4.16	-3.19	-3.47	-2.36
r2b	-2.97	-1.85	-3.27	-2.08	-3.71	-2.68
r2e	-3.40	-2.20	-3.38	-2.30	-2.26	-1.11
r2f	-2.27	-1.02	-3.23	-2.07	-3.39	-2.22
t4b	-2.75	-0.83	-4.27	-2.84	-3.17	-1.56
t4c	-2.81	-1.22	-3.69	-2.21	-3.43	-1.85
t4g	-3.20	-1.48	-2.99	-1.12	-4.31	-2.68
t4h	-2.87	-1.00	-3.79	-2.14	-3.18	-1.37
t4i	-2.39	-0.71	-2.84	-1.13	-2.88	-1.20

Table 2

Binding energy results for three orientations of the C_{82} cage within each configuration in electron volts. Results are ordered such that those on the left contain the least pentagons in the region surrounding that which bonds to the surface and those on the right contain the most.

	Orientation 1		Orientation 2		Orientation 3	
Configuration	Binding energy	Change	Binding energy	Change	Binding energy	Change
r2a	-3.19	0.157	-2.39	0.288	-2.36	0.285
r2b	-2.68	0.202	-2.08	0.217	-1.85	0.247
r2e	-2.30	0.154	-2.20	0.303	-1.11	0.283
r2f	-2.22	0.181	-2.07	0.226	-1.02	0.180
t4b	-2.84	0.143	-1.56	0.247	-0.83	0.174
t4c	-2.21	0.160	-1.85	0.268	-1.22	0.108
t4g	-2.68	0.236	-1.48	0.330	-1.12	0.241
t4h	-2.14	-0.330	-1.37	0.061	-1.00	0.122
t4i	-1.20	0.180	-1.13	0.191	-0.71	0.240

Table 3

Binding energy results for three orientations of the C_{82} cage within each configuration in electron volts. Results are ordered such that binding energies are highest to the left of the table and lowest to the right. In the columns next to the binding energies is the difference between the ratios of the negative eigenvalues in the isolated C_{82} cage and the respective surface configuration.