

THE PENNSYLVANIA STATE UNIVERSITY  
SCHREYER HONORS COLLEGE

DEPARTMENT OF PHYSICS

ELUCIDATING THE EQUILIBRIUM STATE OF C60 MOLECULES ON Ag(111)

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A thesis  
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with honors in Physics

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## ABSTRACT

We have used scanning tunneling microscopy (STM), low-energy electron diffraction (LEED), and density functional theory (DFT) to elucidate the structure and thermodynamics of the  $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$  phase of  $C_{60}$  on Ag(111), which consist of a mixture of two different states/orientations. The structure analysis identifies the orientation of the two types of molecules as  $-C_{60}$  sitting on a vacancy of Ag(111) substrate with hexagon face down and  $C_{60}$  sitting on the top site of Ag(111) surface with its C-C bond down. The molecules flip between two states at a temperature dependent rate. The dynamic of flipping involves the diffusion of the vacancies on Ag(111) surface, producing spatial and temporal correlation of the flipping events. By performing the study with STM, LEED, and DFT, we found the energy difference between two states to be 0.07 eV and the barrier to be 0.84 eV.

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## Chapter 1

### Introduction

Fullerene-based molecular crystals and films are interesting due to their electronic properties such as superconductivity with high critical temperatures ferromagnetism and metal-insulator transitions.<sup>1</sup> They are widely used in electronics devices. The conductance through C<sub>60</sub> molecules on crystal surfaces is strongly dependent on their orientation on the surfaces<sup>2-6</sup>, their surface adsorption site<sup>7</sup>, and their densities<sup>8</sup>. The covalent bonding between the substrate and the adsorption of the C<sub>60</sub> molecules give rise to the conductance of the system<sup>9-12</sup>.

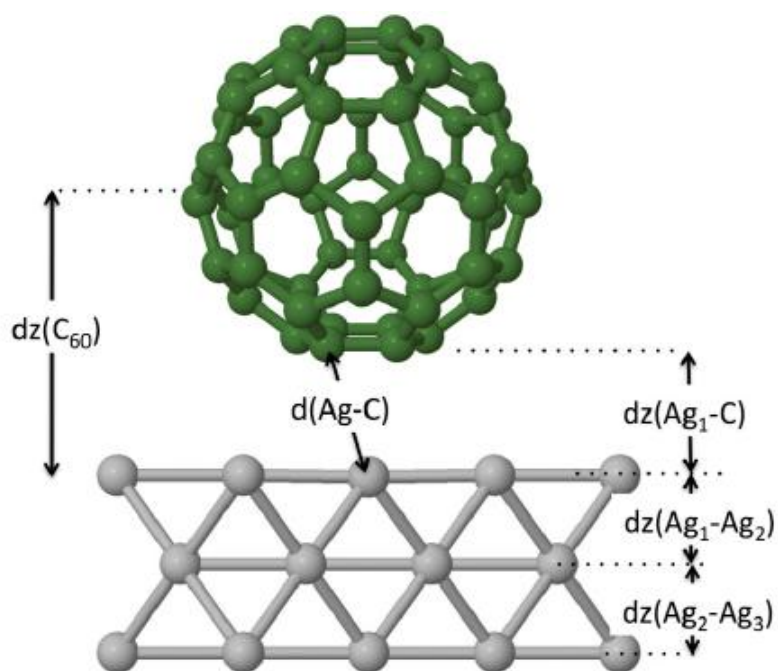
## Chapter 2

### Experiment

To gain insight of the interaction between  $C_{60}$  and the substrate, we performed STM studies to learn the interface between  $C_{60}$  molecules and the substrate. The preparation of the  $C_{60}$  on Ag(111) phase  $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$  was established by dosing the Ag(111) surface with  $C_{60}$  at room temperature, followed by annealing the material for several minutes at  $400^\circ\text{C}$ . After the dosing, most of the  $C_{60}$  film was incommensurate<sup>13,14</sup>; therefore, the annealing process was required. The heating process also desorbed any excess  $C_{60}$  molecules leaving a monolayer of  $C_{60}$  molecules on the surface.

The scanning tunneling microscope (STM) studies materials by imaging their surfaces at the atomic level. Earlier STM studies on an annealed  $C_{60}$  monolayer on Ag(111) showed the surface to have a randomly mixed phase of  $C_{60}$  molecules with “bright” and “dim” contrast in a commensurate superstructure of Ag(111) with a  $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$  unit cell at room temperature. Furthermore, the  $C_{60}$  molecules flip between two states<sup>14,15</sup>. High-resolution STM images at low temperature identified the bright and dim of  $C_{60}$  molecules as corresponding to the orientation with hexagonal site face down (hex) and 6:6 C-C bond down (6:6) respectively.<sup>16</sup> The recent low-temperature low energy electron diffraction (LEED) study suggested that the hex molecules sit on single atom vacancies, which result from the Coulomb repulsion between the ionic bond interaction between  $C_{60}$  and certain closed-pack metal surfaces<sup>9,10,17-19</sup>. Figure 1 illustrates one  $C_{60}$  molecule sitting on top of the Ag(111) surface.





**Figure 1. A hex down  $C_{60}$  molecule sitting on the top side of Ag(111) surface<sup>20</sup>**  
 Distances between the  $C_{60}$  molecule and interdistance between Ag(111) crystals are illustrated in the graph.  $dz$  is the distance between the  $C_{60}$  to the surface.  $d(\text{Ag-C})$  represents the nearest neighbor distance, and  $dz(\text{Ag}_1\text{-C})$  indicates the distance between the first atom in the parenthesis to the second atom in the parenthesis.

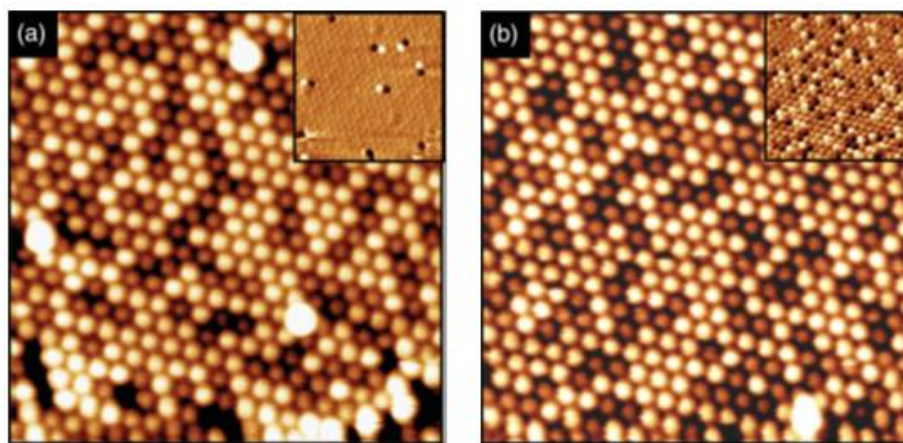
In this study, we used a combination of STM, LEED, and DFT to verify that the hex and 6:6 molecules on Ag(111) adsorb in vacancy and top site, respectively. Successive images were taken through the STM scanning, and we observed “flipping” activities of  $C_{60}$  molecules rotating on top of the substrate. Each image is separated by the time of 43 seconds, which is limited due to the scanning speed of the STM.

## Chapter 3

### Results and Discussion

By studying the images of  $C_{60}$  on the Ag(111) phase  $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$  taken consecutively from the Omicron variable-temperature STM from 295K to 333K, we observed four things – the flipping rate from bright to dim is the same as that of dim to bright; the flipping rate is temperature dependent; flips from bright to dim are correlated to nearby flips from dim to bright; the ratio of the numbers of bright and dim depends on temperature.

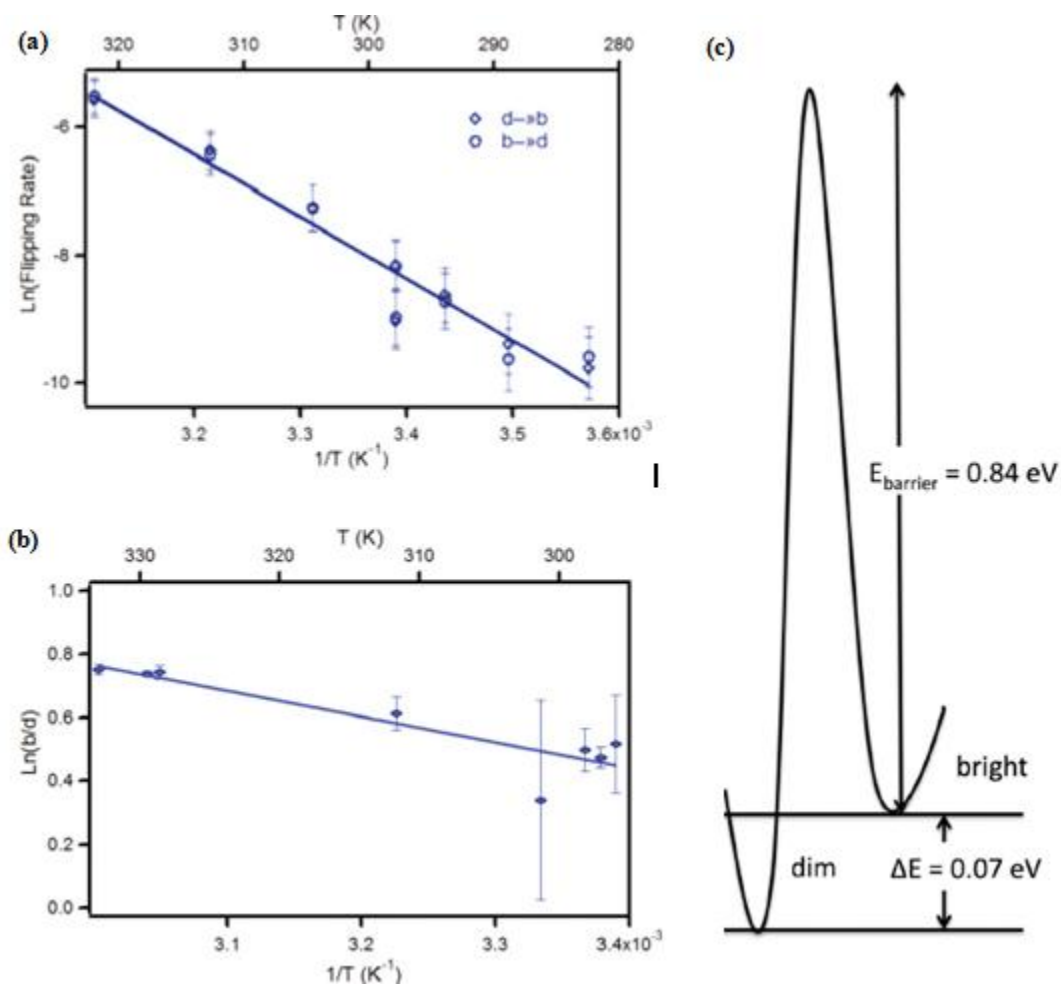
Figure 2 shows the STM images at sample temperatures of 295K and 333K. The insets illustrate the difference between two consecutive images, separated by the frame of 43 seconds – we can observe the events of flipping between bright and dim occur close to their nearby molecules. There exists some superbright molecules in the images, which we believe are the minority species comprising 1%-3% of the molecules due to the surface strain.



**Figure 2. STM  $C_{60}$  image<sup>20</sup>**

Each circle represents a  $C_{60}$  molecule. The insets show the difference between two consecutive frames, separated by 43s. A dark spot indicates the flips from bright to dim and the bright spot correspond to the flip from dim to bright. (a)  $20 \times 20 \text{ nm}^2$  STM image of Ag(111)- $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$  at  $T = 295\text{K}$  and tunneling parameters  $I = 0.06 \text{ nA}$ ,  $V = +1.2\text{V}$ . (b)  $20 \times 20 \text{ nm}^2$  STM image and tunneling parameters  $I = 0.07 \text{ nA}$ ,  $V = +2.2\text{V}$ .

By studying the images of the dynamics of  $C_{60}$  molecules, we observed that both the flipping rate and the bright to dim ratio of  $C_{60}$  molecules are correlated to the temperature change. Figure 3 below shows the semi-log plot of the event dependency on temperature. The slopes of the semi-log plot of flipping rate and bright to dim ratio versus inverse temperature corresponds to the energy barrier and energy difference between the bright and dim states. We found the energy barrier to be  $0.84 \pm 0.05$  eV and the energy difference to be  $0.07 \pm 0.02$  eV.

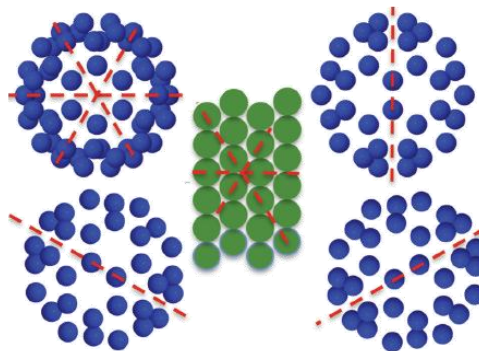


**Figure 3.  $C_{60}$  two-state system**

(a) Semi-log plot of the flipping rate versus inverse temperature. The slope corresponds to the activation energy of  $0.84 \pm 0.05$  eV. (b) Semi-log plot of the bright to dim ratio as a function of inverse temperature. The slope represents the energy difference between two states:  $0.07 \pm 0.02$  eV. (c) Schematic of the bright-dim two-state system

From Figure 3 (a), we note that at the same temperature, the flipping rate from dim to bright is essentially the same as that from bright to dim, which indicates the system to be at equilibrium. The occurrence of flipping events is in proportion to the temperature. The temperature range in this experiment is limited by the scanning speed of the STM and the kinetics of the flipping. At lower temperature, the flipping occurs too slowly so that it would take hours for the system to reach the equilibrium. On the other hand, at higher temperature, the flipping rate is too fast between each frame (43s apart) that we could not accurately measure the flipping rates. Figure 3 (b) illustrates the bright to dim ratio of the system with temperature dependence. The ratio of bright to dim is proportional to the temperature, showing the dim state to be a more preferable stable state.

We have observed the spatial adjacency of the flipping events. In order to understand more detail of this activity, we carried out LEED and DFT study of to obtain more geometrical details of  $C_{60}$  molecules. The earlier LEED experiment was performed at  $T = 32K$ .<sup>21</sup> The diffraction intensities shown here were treated as an incoherent sum of two types of  $C_{60}$  molecules due to the randomness of the spatial distribution and optimization of the fit. We only allowed variation in the optimization of the perpendicular coordinates to the surface in order to reduce the computational burden of the testing of all possibilities of the configuration. Figure 4 shows the symmetry of two orientations of  $C_{60}$  molecules of on the Ag(111) surface. The hex molecules are aligned with their mirror symmetry planes parallel and anti-parallel to the that of the Ag(111) substrate. The 6:6 molecules have three equivalent orientations and it is not possible to distinguish between the orientations from the STM at this point. The mirror planes of the 6:6 molecules are  $30^\circ$  from the substrate mirror planes.



**Figure 4. Two types of  $C_{60}$  on  $Ag(111) (2\sqrt{3} \times 2\sqrt{3})R30^\circ$  surface found in high-resolution STM images.**  
 The center panel shows the top surface of the  $Ag(111)$  substrate. Red dashed lines indicate the mirror planes of the symmetry.  $C_{60}$  molecules have two phases – hex and 6:6. There are two orientations (parallel and antiparallel) in hex but three possible orientations in 6:6.

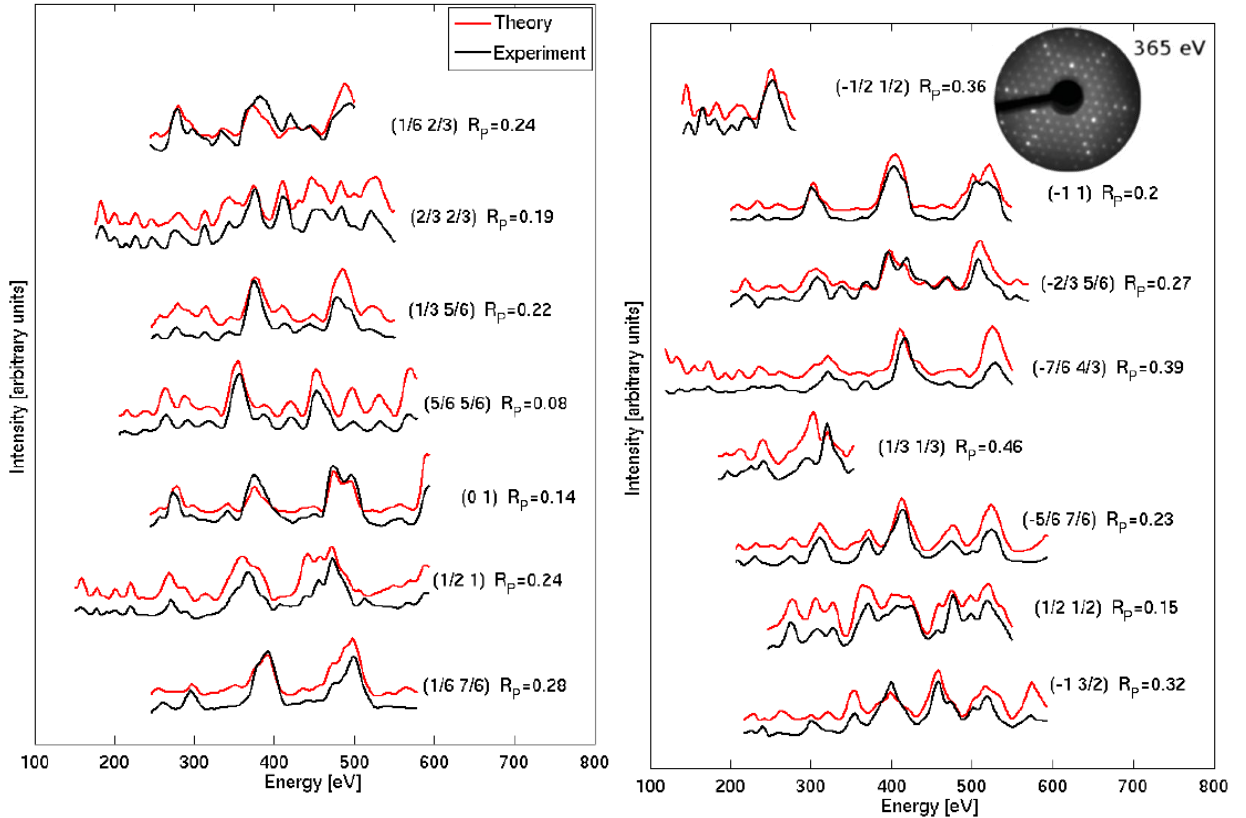
By performing LEED analysis, we can extract the intensities of the diffraction spots from the experiment and obtain the  $I(E)$  curves to compare with the calculated models. Since there is symmetry of the molecules and the substrate, we averaged the intensity curves while comparing them with the calculated models. The calculation was done by using SATLEED<sup>24</sup> and LEEDFIT<sup>25</sup> codes. The proximity of the calculated spectra can be compared with the measured data by the Pendry  $R$  factor<sup>23</sup>, which has a value of 0 for identical spectra and 1 for no correlation. We managed to eliminate orientations other than top and vacancy sites of the adsorption from the fact of the  $R$  factors were greater than 0.7 for the first trial run. We also excluded the models with  $R$  factor greater than the optimum  $R$  factor +  $RR$ , the variance of the Pendry  $R$  factor. The test of  $R$  factors for different configurations of  $C_{60}$  on  $Ag(111)$  were in the range of 0.34-0.40. The test was performed on a mixture of hex and 6:6, sitting on different sites of the substrate. The results showed an improvement on the agreement with the experimental data. After mixing the hex and 6:6, the  $R$  factors were between 0.24 and 0.28, and the  $RR$  factor was 0.02. Therefore, models having  $R$  factor  $> 0.28$  are very unlikely to correspond to the true structure. Table I below includes the  $R$  factors of models with different constrains. The best result for  $T = 32K$  is 50:50 mixtures of hex-vac and 6:6:-top molecules. The results also show the hex molecules to have

50:50 mixtures of mirror planes parallel and anti-parallel to that of the substrate and 6:6 molecules to have equally distributed 3-fold orientation and  $30^\circ$  angle difference to the substrate.

Figure 5 below shows the spectrum of the experimental and calculated  $I(E)$  curves.

**Table I. Pendry R factors obtained from the specified mixture of C<sub>60</sub> molecules on Ag(111)**  
Hex and 6:6 represent the hexagon-down and C-C bond down orientation respectively; top and vac refers to the adsorption site of top and vacancy on the Ag(111) surface respectively. The angles indicate the degree difference of the mirror planes between the molecules and the substrate. The best fit configuration is 50:50 hex-vac to 6:6-top, with  $R$  factor = 0.24.

C <sub>60</sub> /Ag(111)	Hex-top	Hex-vac	6:6-top	6:6-vac
Incoherent mixing	(0° + 180°)	(0° + 180°)	(30°)	(30°)
Hex-top (0° + 180°)	0.35	0.34	0.25	0.28
Hex-vac (0° + 180°)	0.34	0.34	<b>0.24</b>	0.28
6:6-top (30°)			0.37	
6:6-vac (30°)				0.40



**Figure 5. Representative LEED spectra and LEED pattern for C<sub>60</sub> molecules on top of Ag(111).**

The numbers in the parameters correspond to the Miller indices of the diffraction pattern. The experiment was performed using 15 beams with total energy of 4860 eV. The full set of data can be found at the Appendix A. Numerical data can be found at Phys. Rev. B **86**, 205406

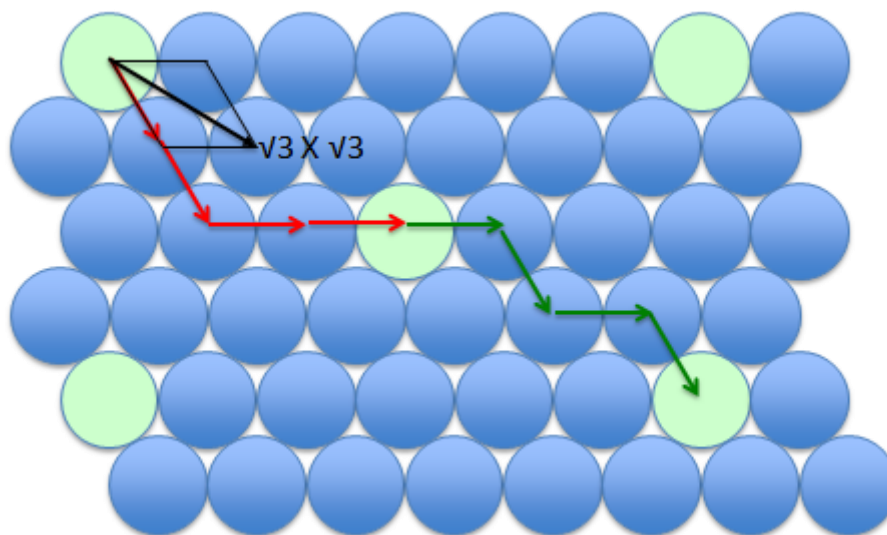
Table II gives the information of  $C_{60}$  molecules structure on Ag(111) determined by LEED, where the parameters refer to Figure 1. For both hex and 6:6 structures, there exist small relaxations of the atoms closest to the molecules. But very little deformation of the  $C_{60}$  molecules, which presumably is due to the large energy cost to deform the C-C bond compared to  $C_{60}$ -Ag bond.

**Table II. Best-fit parameters of  $C_{60}$  on Ag(111) according to the LEED analysis.**

All the units are in Å. The parameters are corresponded to that shown in Figure 1.  $dz(C_{60})$  is the distance between the center of the molecules to the top surface;  $d(\text{Ag-C})$  represents the distance between the first atom (Ag) to the second atom (C);  $\Delta$  corresponds to the average interlayer distance between each planes of the substrate.

Parameter	Hex-vac	6:6 - top
$dz(C_{60})$	$5.2 \pm 0.1$	$5.5 \pm 0.1$
$d(\text{Ag-C})$	$2.5 \pm 0.1$	$2.1 \pm 0.1$
$dz(\text{Ag}_1\text{-C})$	$2.0 \pm 0.1$	$2.0 \pm 0.1$
$dz(\text{Ag}_1\text{-Ag}_2)$	$2.35 \pm 0.03$	$2.34 \pm 0.04$
$dz(\text{Ag}_2\text{-Ag}_3)$	$2.34 \pm 0.04$	$2.34 \pm 0.05$
$dz(\text{Ag}_3\text{-Ag}_4)$	$2.35 \pm 0.06$	$2.34 \pm 0.06$
$\Delta_1$	$0.03 \pm 0.03$	$0.05 \pm 0.04$
$\Delta_2$	$0.02 \pm 0.04$	$0.06 \pm 0.05$
$\Delta_3$	$0.03 \pm 0.05$	$0.05 \pm 0.06$

In terms of the spatial correlation of the flipping events, at stated earlier, we found the flipping activities occur mainly between neighbors. Since we have investigated the structure is hex-vac and 6:6-top, when the flipping happens, the Ag atom at the top site will transfer to the nearby vacancy site; for instance, the movements of the Ag atoms underneath the molecules give rise to the flipping activities. The diffusion barrier for a vacancy on Ag(111) has been calculated using surface embedded atom method to be 0.404 eV, compared the flipping barrier of 0.84 eV.<sup>26</sup> However, we note that when a flip occurs, there are several diffusion paths the atom can take. If the flip is from site to site, there would be at least four hops on the Ag(111) surface. Figure 6 shows the diffusion paths and the top view of  $C_{60}$  molecules on Ag(111) surface.



**Figure 6. Top view of  $C_{60}$  molecules in a  $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$  Ag(111) structure.**

Each of the bright spot indicates the position of a  $C_{60}$  molecule. Each dark atom represents an Ag atom. The black arrow shows a  $(\sqrt{3} \times \sqrt{3})R30^\circ$  structure; since we study  $(2\sqrt{3} \times 2\sqrt{3})R30^\circ$  structure, the distance is doubled between two molecules. Red and green arrows indicate possible path for a Ag atom. From the illustration of the model, we can see in order to get to the next molecule; Ag atoms are going to undergo at least four hops.

To understand the relative energetics, we performed DFT studies<sup>21,27</sup>. We looked at the  $(4\sqrt{3} \times 2\sqrt{3})R30^\circ$  surface to include two  $C_{60}$  molecules to explore the effects of multiple molecules orientations. Table III indicates the adsorption energy for different  $C_{60}$  molecule orientation and configuration.

**Table III. Calculated adsorption energy per molecule for various geometric formation of  $C_{60}$  on Ag(111)**

1- $C_{60}$	$E_{ads}$ (eV)	2- $C_{60}$ configuration	$E_{ads}$ (eV)
Hex-vac	1.44–1.74	Hex-vac + hex-vac	1.44–1.74
Hex-top	1.20	Hex-vac + hex-top	1.36–1.51
6:6-top	1.27	Hex-vac + 6:6-top	1.40–1.55
6:6-vac	0.94–1.24	Hex-vac + 6:6-vac	1.22–1.52

When a vacancy is formed, the exact location of extracted substrate atom has a significant effect on the adsorption energy in these calculations. Two limiting cases correspond



to the Ag atom allowed to adsorb on top of the surface, and the Ag atom taking a lattice site in the bulk of the crystal. The results from Table III shows that the hex-vac is more favorable than the hex-top orientation, and 6:6-top is preferred than 6:6-vac. As we extended the DFT to include two  $C_{60}$  molecules, the results did not change compared to single  $C_{60}$  molecules, implying the mutual molecular orientation of neighbors does not strongly affect the adsorption site. These results, along with the temperature dependence of the flipping rate and the bright to dim ratio, lead us to the conclusion of the mixing of  $C_{60}$  molecules on Ag(111) is entropic.

## Chapter 4

### Conclusion

We have measured the equilibrium configuration of  $C_{60}$  molecules in the Ag(111) phase ( $2\sqrt{3} \times 2\sqrt{3}$ ) $R30^\circ$ . The results indicate that the orientation of two species of  $C_{60}$  molecules sitting on Ag(111) are with hexagon-down (hex) sitting on the vacancy site of the substrate and C-C bond down (6:6) locating on the top site of the surface. Hex site has mirror planes parallel and anti-parallel to the mirror planes of the substrate while 6:6 have 3-fold symmetry with mirror planes  $30^\circ$  differ from the substrate. From the study of flipping rate and bright to dim ratio of  $C_{60}$  molecules, we concluded that the activation energy barrier between the two states of  $C_{60}$  is  $0.84 \pm 0.05$  eV and the energy difference between the states is  $0.07 \pm 0.02$  eV. The hex-vac is the lower energy state and 6:6-top is the higher energy state. We have gained the insight into the nature of the flipping events of  $C_{60}$  molecules on Ag(111) surface. Future work can be done on similar substrate of Au(111) or other surfaces to understand fullerene properties in order to gain an understanding that can be applied to industrial products.

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- Awarded Lane Granville B Memorial Scholarship 2012-13
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- Awarded Schraer Harald Scholarship for Women 2011-12
- Awarded George E. Sperling and Elizabeth S. Sperling Trustee Scholarship *Eberly College of Science*  
*The Pennsylvania State University*  
2010-11
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## Professional Experience

- **REU at University of California, Los Angeles** *University of California, Los Angeles*  
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  - Simulated properties of plasma particles in thermal equilibrium using PIC codes and gridless code
  - Used C++ on algorithm operation of the data
  - Plotted data points using gnuplot
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*Department of Physics*

- Presented *NISXW Study of Si adsorbed on an Al-Co-Ni Quasicrystal* at the ICSOS-10 (10<sup>th</sup> International Conference of Structure of Surface) — Hong Kong, Aug. 1- Aug. 5, 2011
- Studied the dynamical equilibrium of C<sub>60</sub> molecules on Ag(111)
- Used Jmol software to understand crystal structure in atomic scale
- Extracted intensity of LEED pattern from HotLEED program
- Worked on Au(111) surface and Si on W approximation
- Maintained research website

## **Research Interests**

I have broad interests in science and engineering, in particularly the applied science. Currently, I am interested in particle physics and applied physics. I decide to continue physics studies in PhD and hoping to obtain a job in national laboratory.

## **Professional Presentations**

- S. Su, *et al.* “Elucidating the Dynamic Equilibrium of C<sub>60</sub> Molecules on Ag(111)”, American Physics Society March Meeting, Baltimore, Mar. 18 – Mar. 22, 2013
- S. Su, *et al.* “Verification and Convergence Study of Particle-in-Cell (PIC) Codes”, 54<sup>th</sup> American Physics Society Plasma Division Meeting, Providence Rhode Island, Oct. 29 – Nov. 2, 2012
- S. Su, *et al.* “NISXW Study of Si adsorbed on an Al-Co-Ni Quasicrystal”, ICSOS-10 (10<sup>th</sup> International Conference of Structure of Surface), Hong Kong, Aug. 1- Aug. 5, 2011

## **Publications and Papers**

- K. Pussi, H. I. Li, H. Shin, L. N. Serkovic Loli, A. K. Shukla, J. Ledieu, V. Fourné, L. L. Wang, S. Y. Su, K. E. Marino, M. V. Snyder and R. D. Diehl, "Elucidating the Dynamical Equilibrium of C<sub>60</sub> Molecules on Ag(111)", *Phys. Rev. B* 86, 205406 (2012).