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Photoelectron spectra calculations of N@C$_{60}$ molecules on a crystalline Si surface

A. S. Baltenkov,[1,2,3] U. Becker,[4] S. T. Manson,[1] and A. Z. Msezane[2]

[1]*Department of Physics and Astronomy, Georgia State University, Atlanta, Georgia 30303, USA*
[2]*Center for Theoretical Studies of Physical Systems, Clark Atlanta University, Atlanta, Georgia 30314, USA*
[3]*Arifov Institute of Electronics, 700125, Tashkent, Uzbekistan*
[4]*Fritz-Haber-Institute der Max-Planck-Gesellschaft, 14195 Berlin, Germany*

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The shapes of the angular distributions of electrons photoejected from the 1*s* level of atomic N encapsulated within a fullerene cage have been calculated for N@C$_{60}$ adsorbed on a Si (100) crystal surface. Two possible schemes of experimental arrangements have been considered. The first involves the measurement of the photoelectron spectra as a function of the polar angle for fixed azimuthal angle. The second scheme studies the dependence of the spectra on the azimuthal angle. It is shown that in both types of experiments the shape of the photoelectron angular distribution is extremely sensitive to both the molecular location on the crystal surface and the orientation of the molecular axis of the fullerene cage relative to crystallographic directions. Therefore, the study of photoelectron spectra can, in principle, be used for diagnostics of the position of the fullerenelike molecule on a crystal surface.

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I. INTRODUCTION

The present paper is devoted to the theoretical investigation of the photoelectron spectra of N@C$_{60}$-doped fullerenes positioned on a Si crystal surface. The interest in these surface structures is connected with the possibility of using them to create quantum information processing devices (see, for example, Ref. 1 and references therein). These doped N atoms are paramagnetic due to their half-filled *p* subshells, and for this reason they are interesting in connection with the possibility of electron-spin quantum computation. The placing of the N atoms inside the highly symmetric fullerene cage eliminates the contribution of any anisotropic interactions and efficiently suppresses the broadening of the electron-spin resonance lines. Extreme narrowness of these lines together with the long spin lifetime makes these doped fullerenes attractive candidates for quantum computation devices.

The monolayer formation of N@C$_{60}$ molecular or endohedral fullerene chains on the Si crystal surface can be used for storage and manipulation of quantum information. The endohedral fullerenes can be individually positioned on the Si crystal.[2] The problem is to control their positions—i.e., place them in an orderly arrangement. Here we investigate the possibility of exerting this control through the photoelectron angular distribution resulting from the photoionization of the encapsulated N atoms in N@C$_{60}$ molecules adsorbed on the Si crystal surface. In our previous papers[3,4] devoted to the photoionization of endohedral atoms, it was shown that the angular distribution of photoelectrons emitted by inner-shell photoionization of an atom inside a C$_{60}$ cage is extremely sensitive to the positions of the atoms surrounding the encapsulated atom. There are reasons to believe that the shapes of the photoelectron spectra for adsorbed endohedral molecules will be sensitive to the positions of the silicon substrate atoms. Information on the position of the endohedral molecule on the Si crystal surface, apparently, can be extracted from photoelectron spectra, and for this reason the corresponding theoretical description of the photoionization process is of great utility.

The calculation of the photoelectron spectra, involving the 61 atoms of the N@C$_{60}$ system *plus* the many nearby Si atoms on the surface, is extremely complicated. To render the calculation more tractable, several simplifying, but physically reasonable, approximations are made. First, it is assumed that the endohedral fullerenes are rigidly fixed on the crystal surface. It is further assumed that the A@C$_{60}$ fixing on the substrate is due to physical adsorption (physisorption) and is not accompanied by chemical transformation of the molecules themselves. Therefore, we neglect the deformation of the C$_{60}$ cage because of its interaction with both the substrate and encapsulated atom itself. This assumption is quite reasonable in view of the extremely low reactivity of C$_{60}$. Earlier theoretical work[5] showed that the exchange interaction between neighboring endohedrals on the surface, either directly by contact or mediated by a substrate, is vanishingly small. This allows us to consider the photoionization of the surface structures as an ionization process of a separate molecule on the crystal surface. In addition, it is assumed that the adsorbed C$_{60}$ cages and atoms inside them are positioned in a strongly defined manner relative to the single-crystal surface and, hence, relative to the polarization vector of the radiation. We do not consider any effects connected with the possible migration of the encapsulated atom to the inner surface of the cage; in N@C$_{60}$, the N atom resides at the center of the fullerene without any charge transfer to the C$_{60}$ cage.[6] Therefore, such effects are generally weak and can be neglected.

II. MAIN FORMULAS

The formulas employed in this paper have been derived earlier,[3,4,7] so here we present only the main ones. In the photoionization of a deep subshell of the A atom in the system A@C$_{60}$+(Si surface), the initial state of the 1*s* electron of the A atom is described by the usual wave function of this atom. Therefore, it is necessary to take into account the presence of the 60 carbon atoms of the C_{60} cage and the surface Si atoms to construct the wave functions of the continuum only. For the molecular continuum calculations we apply the methodology developed previously.[7] While studying the photoionization of free endohedral fullerenes,[3,4] we considered photoelectron scattering only by the carbon atoms forming the C_{60} cage. For photoionization of the adsorbed endohedral fullerene, besides photoelectron scattering by the C_{60} atoms, the scattering by the substrate Si atoms becomes important. Therefore, we consider the potential field of the C_{60}+Si system as a superposition of nonoverlapping potentials of the C and Si atom scatterers. We represent the continuum wave functions using linear combinations of the Green's functions of the Schrödinger equation for the ionized A atom with the hole in the $1s$ subshell. The coefficients of this linear combination are defined by the boundary conditions imposed on the wave function at the points of the localization of the C and Si atoms. Constructed in such a way, the wave function far from the $A@C_{60}$+Si system has the form of a superposition of the spherical waves emitted both by the ionized A atom and by each of the C and Si atom scatterers; i.e., it has the correct asymptotic behavior. This is extremely important for the correct description of the photoelectron angular distribution.

In atomic units ($\hbar = m = e = 1$) used throughout this paper, the angular distribution of the electrons photoejected from the deep s level of the A atom in the presence of the fixed-in-space atom scatterers near threshold is give by[3,4]

$$\frac{d\sigma(\omega)}{d\Omega} = \frac{3}{4\pi}\sigma_A(\omega)S(\mathbf{k}). \tag{1}$$

Here $\sigma_A(\omega)$ is the total photoionization cross section of the $1s$ level of the free A atom, ω is the photon energy, and $\mathbf{k} = k\mathbf{n}$ is the photoelectron momentum. According to Eq. (1), the differential photoionization cross section is a product of two dynamical factors. The first, $\sigma_A(\omega)$, depends on the bound and continuum wave functions for the free A atom, whereas the second, referred to as a structural function $S(\mathbf{k})$, defined as

$$S(\mathbf{k}) = \left| (\mathbf{e}\cdot\mathbf{n}) + ie^{-i\Delta_1}\frac{k}{2\pi}\sum_{j=1}^{60+N} C_j^+(-\mathbf{k})\chi_{k1}^+(R_j)(\mathbf{e}\cdot\boldsymbol{\rho}_j) \right|^2, \tag{2}$$

depends on the molecular structure. Here $\mathbf{e}$ is the photon polarization vector, the vectors $\mathbf{R}_j$ define the positions of the nuclei of the 60 C atoms of the fullerene cage and the N Si atoms in the coordinate system whose origin is at the nucleus of the A atom, $\boldsymbol{\rho}_j = \mathbf{R}_j/R_j$ are the corresponding unit vectors, $\chi_{k1}^+(R_j) = i\varphi_{k1}(R_j) - \chi_{k1}(R_j)$ are the linear combination of the regular $\varphi_{k1}(R_j)$ and irregular $\chi_{k1}(R_j)$ solutions of the radial Schrödinger equation for the photoelectron (with orbital angular momentum $l=1$) moving in the field of the A atom with the hole in the $1s$ subshell, and $\Delta_1(k)$ are the phase shifts of these wave functions. The coefficients $C_j^+(-\mathbf{k})$ are the solutions of a system of nonhomogeneous linear equations

$$C_j^+(-\mathbf{k}) - 2\pi f_j \sum_{i\neq j}^{60+N} C_i^+(-\mathbf{k})G_k^+(\mathbf{R}_i,\mathbf{R}_j) = 2\pi f_j \psi_{-\mathbf{k}}^+(\mathbf{R}_j),$$

$$j = 1,2,\ldots,60+N, \tag{3}$$

where $f_j = (e^{2i\delta_j} - 1)/(2ik)$ are the s-wave amplitudes for photoelectron scattering by the C atoms (for $j = 1,\ldots,60$) and by the Si atoms (for $j = 61,\ldots,60+N$) and the $\delta_j(k)$ are the corresponding s-wave phase shifts. The $G_k^+(\mathbf{R}_i,\mathbf{R}_j)$ are the Green's functions of the Schrödinger equation for a photoelectron moving in the field of the ionized A atom. The wave functions $\psi_{\mathbf{k}}^+(\mathbf{r})$ in Eq. (3) are given by the familiar formula[8]

$$\psi_{\mathbf{k}}^+(\mathbf{r}) = 4\pi\sum_{l,m} i^l e^{i\Delta_l} Y_{lm}(\mathbf{r}) Y_{lm}^*(\mathbf{k})\varphi_{kl}(r). \tag{4}$$

Here, the spherical harmonics $Y_{lm}(\mathbf{r}) \equiv Y_{lm}(\Omega)$ and $Y_{lm}(\mathbf{k}) \equiv Y_{lm}(\Omega_k)$ depend on the spherical coordinates of the vectors $\mathbf{r}$ and $\mathbf{k}$, respectively. Formulas (1)–(4) will be utilized to calculate the function $S(\mathbf{k})$ for the $1s$ photoionization of the nitrogen atoms in the $N@C_{60}$+Si system.

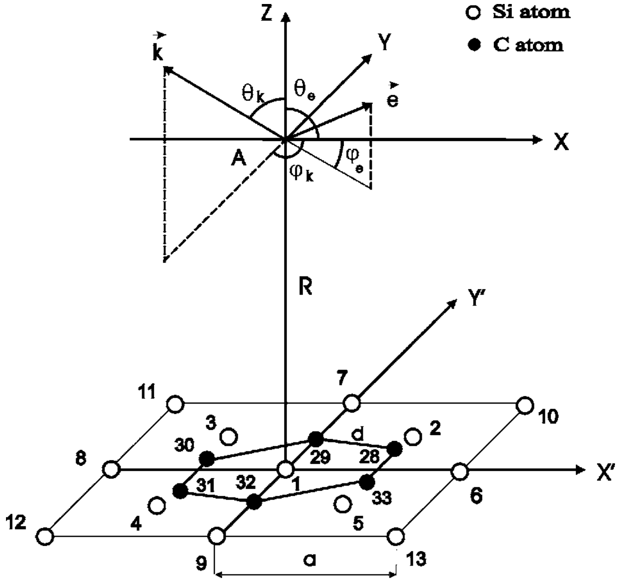

FIG. 1. Geometry of the positions of the N atom, 6 C atoms (28-29-30-31-32-33) of the C_{60} cage and 13 Si atoms for the $N@C_{60}$ molecule on the (100) crystal surface. The N atom is located at point A. Distances a and d are the lattice constant and the bond length of the C_{60} hexagon, respectively. The azimuthal angles φ_e, φ_k, and φ_j are measured from the X axis toward the Y axis, counterclockwise, viewing the surface from point A.

III. GEOMETRY OF THE SYSTEM $A@C_{60}$+Si

We have previously calculated[3] the spherical coordinates of the vectors $\mathbf{R}_j$ defining the position of the C atoms of the C_{60} cage in the coordinate system with the origin at the center of this cage (where, in the given case, the trapped atom is located) and the Z axis that goes from the middle of the two opposite hexagons of the C_{60} cage (see Fig. 1 of Ref. 3). These coordinates, the $\mathbf{R}_j$ structure of the C_{60} cage,[3] are used to investigate the $A@C_{60}$ molecule resting on the hexagon

TABLE I. The set of spherical coordinates of the vectors $\mathbf{R}_j(R_j, \vartheta_j, \varphi_j)$ of the Si atoms on the (100) crystal surface.

j	R_j	ϑ_j (rad)	φ_j (rad)
1	6.720521	3.141593	0.0
2	9.892740	2.317657	0.785398
3	9.892740	2.317657	2.356194
4	9.892740	2.317657	3.926991
5	9.892740	2.317657	5.497787
6	12.27058	2.150401	0.0
7	12.27058	2.150401	1.570796
8	12.27058	2.150401	3.141593
9	12.27058	2.150401	4.712389
10	15.99903	2.004305	0.785398
11	15.99903	2.004305	2.356194
12	15.99903	2.004305	3.926991
13	15.99903	2.004305	5.497787
14	17.56901	1.963320	0.321751
15	17.56901	1.963320	1.249046
16	17.56901	1.963320	1.892547
17	17.56901	1.963320	2.819842
18	17.56901	1.963320	3.463344
19	17.56901	1.963320	4.390638
20	17.56901	1.963320	5.034140
21	17.56901	1.963320	5.961434
22	22.79197	1.870109	0.785398
23	22.79197	1.870109	2.356194
24	22.79197	1.870109	3.926991
25	22.79197	1.870109	5.497787

with vertexes 28-29-30-31-32-33 upon the Si (100) surface. First, we assume that the A atom being ionized is located on the normal to the (100) surface of the Si crystal directly over one of the Si atoms at a distance R equal to the C$_{60}$ radius. Figure 1 represents this geometry of the A@C$_{60}$+Si system. In Fig. 1 the (100) plane with 13 neighboring Si atoms and 6 C atoms of the lower pentagon is depicted and the spherical coordinates of the photon polarization vector $\mathbf{e}(\vartheta_e, \varphi_e)$ and the photoelectron wave vector $\mathbf{k}(\vartheta_k, \varphi_k)$ are indicated. In this coordinate system with the center at the ionized atomic nucleus (point A in Fig. 1) and with the polar Z axis directed perpendicular to the crystal surface, the spherical coordinates of the 25 Si atoms located on the (100) plane are given in Table I.

Calculations show that if we restrict ourselves to the consideration of the crystal atoms of the upper layer, then a further increase in the number of the Si atoms in the calculation has no significant impact on the shape of the photoelectron angular distribution. For the calculation of the coordinates of the system it is assumed that the fullerene radius is $R \approx 6.720$ a.u., the distance between the C atoms of the cage is $d \approx 2.722$ a.u.[9] and the Si lattice constant is $a \approx 10.096$ a.u.[10] Along with the spherical coordinates of the C atoms in the C$_{60}$ cage (the $\mathbf{R}_j$ structure[3]), we now have the coordinates of all the 85 atom scatterers for the given position of the A@C$_{60}$ molecule on the surface. The procedure for the numerical solution of Eq. (3) and the calculation of the structural function $S(\mathbf{k})$ are described in detail elsewhere[3,4] and will not be repeated here.

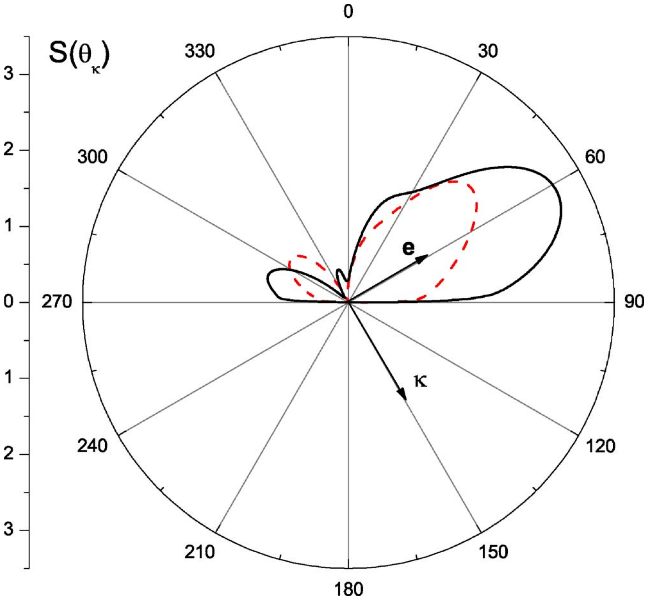

FIG. 2. (Color online) Structural function $S(\vartheta_k)$ for photoelectron emission in the plane XZ. The dashed line corresponds to data for the free N atom near the Si crystal surface at point A, and the solid line is $S(\vartheta_k)$ for N@C$_{60}$ at point A.

IV. RESULTS OF CALCULATIONS

We begin with the case of the center of the C$_{60}$ cage—i.e., the N atom—being over one of the Si atoms as shown in Fig. 1 and calculate the structural function $S(\mathbf{k})$ corresponding to this geometry of the system. Then we shift the molecule to another point of the surface. As a result of these calculations, we obtain the photoelectron spectra for different points of the molecular adsorption on the surface. The differences found in the photoelectron spectra for the molecule adsorbed at various points of the Si surface will provide information on the point of molecular localization on the crystal surface. This will allow, in principle, the control of the A@C$_{60}$ molecular position on the silicon surface. For all calculations the photoelectron wave vector k will be set equal to $k=0.5$ a.u., corresponding to photoelectron kinetic energy $\varepsilon \approx 3.4$ eV and photon energy $\omega = I_{1s} + k^2/2$, where the ionization potential calculated within the Hartree-Fock approximation is $I_{1s} \approx 31.333$ Ry.

A. Polar angle dependence

Consider the photoionization of the 1s level of the N atom by a linearly polarized photon whose wave vector $\boldsymbol{\kappa}$ and polarization vector $\mathbf{e}$ are in the plane XZ. The spherical coordinates of the vector $\mathbf{e}$ are $\mathbf{e}(\vartheta_e = 60°, \varphi_e = 0°)$. To begin with, we investigate how the shape of the photoelectron angular distribution of the isolated N atom changes with successive consideration of the Si atoms of the surface and then the C atoms forming the fullerene cage in addition. In Fig. 2 the calculated structural function $S(\mathbf{k})$ for the

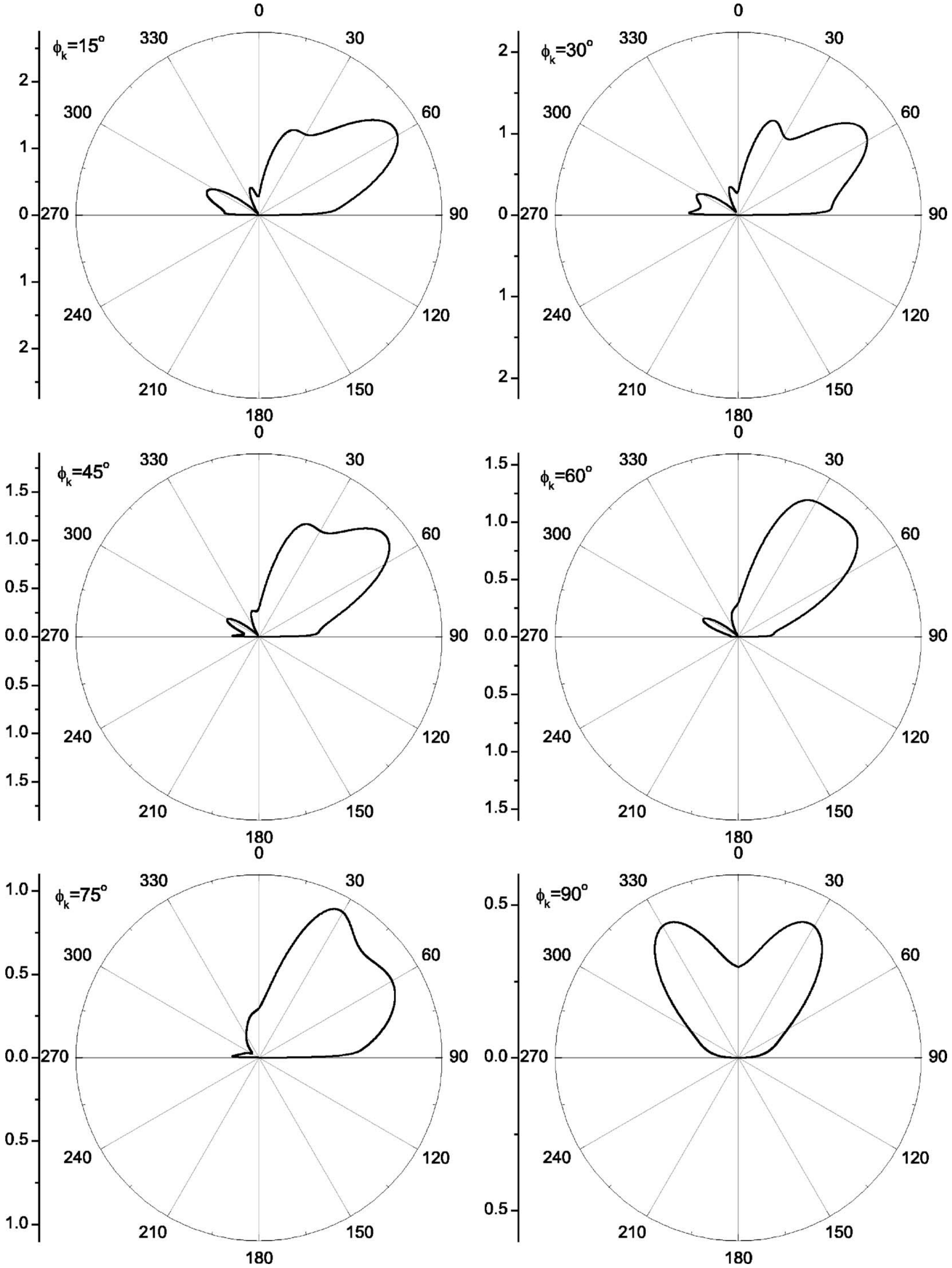

FIG. 3. Structural function $S(\mathbf{k})$ as a function of polar angle ϑ_k for the N@C$_{60}$+(Si surface) system when the N atom is located at the first point of adsorption (see Fig. 1 and text). Each of the figures corresponds to a fixed azimuthal angle φ_k, shown in the upper left corner of each figure.

photoelectrons emitted perpendicular to the crystal surface in the plane *XZ* for the N atom located near the surface at point *A* is presented. In the absence of the Si atom scatterers—i.e., in the case of an isolated N atom—the photoelectron angular distribution in the *XZ* plane has the form $S(\vartheta_k, \varphi_k=0) \sim \cos^2(\vartheta_k - \pi/3)$. The presence of the surface atoms of Si radically changes this shape of the electron angular distribution. In the case of the free atom, the photoelectrons are emitted mainly along the photon polarization vector $\vartheta_k=60°$, but in the field of the Si surface, the maximum emission in the right semiplane *XZ* falls at an angle $\vartheta_k \sim 45°$. In the left semiplane (in Fig. 2 these are the polar angles within the range of 360°–270°) a peak of lesser intensity (dashed line), which is absent in the case of a free atom, appears at $\vartheta_k \sim 310°$. The origin of this second peak is connected with reflection from the crystal surface of the photo-

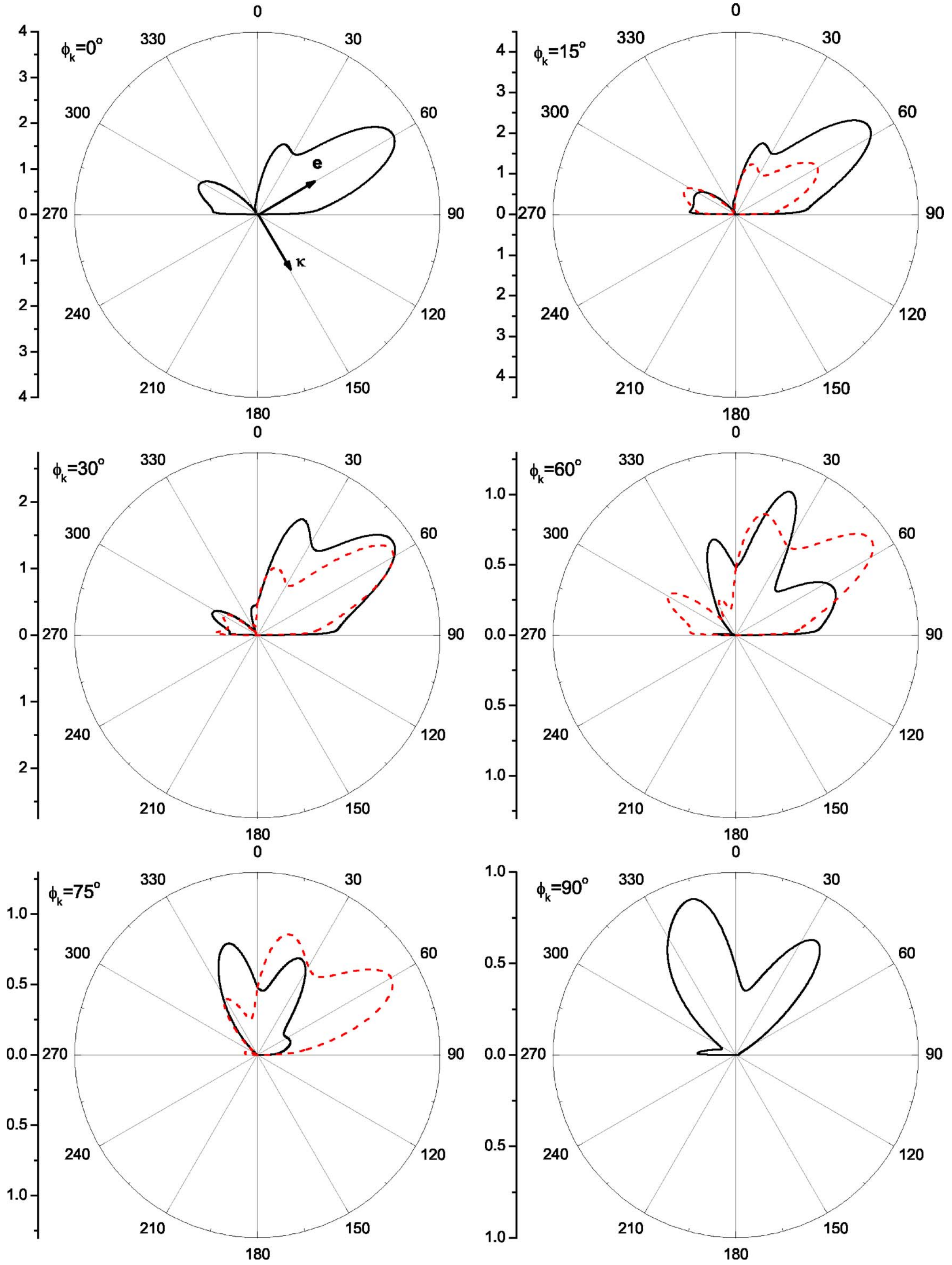

FIG. 4. (Color online) Structural function $S(\mathbf{k})$ as a function of polar angle ϑ_k for the second point of the N@C_{60} molecule adsorption (see Fig. 1 and text). The vectors $\boldsymbol{\kappa}$ and $\mathbf{e}$ are situated in the XZ plane. The solid line corresponds to $S(\mathbf{k})$ for the fixed azimuthal angle φ_k and the dashed line to $S(\mathbf{k})$ for angle 2π-φ_k. The angle φ_k is shown in the upper left corner of the figure.

electrons emitted into the lower semisphere filled with the crystal. The second curve in Fig. 2 (solid curve) corresponds to the photoionization of the N atom being as before at point *A* but encapsulated in the fullerene cage C_{60}—i.e., the molecule N@C_{60}. The main photoemission maximum in this case is shifted, as compared to the previous case, and occurs at an angle $\vartheta_k \sim 60°$. But in the left semiplane, instead of one peak at $\vartheta_k \sim 290°$, a second peak of less intensity (at $\vartheta_k \sim 340°$) appears. Thus, each group of atom scatterers makes a particular contribution to forming the photoelectron

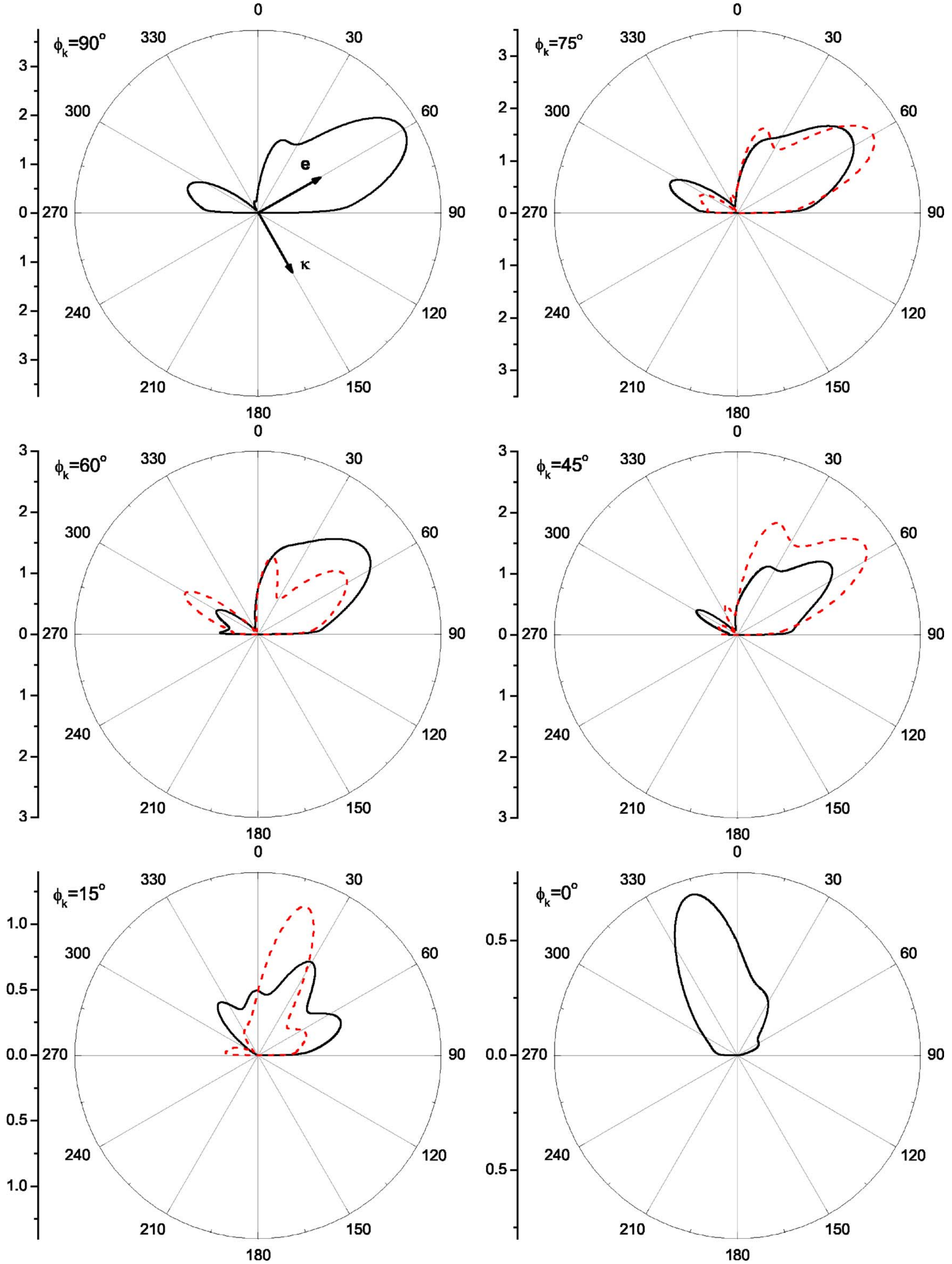

FIG. 5. (Color online) Structural function $S(\mathbf{k})$ as a function of polar angle ϑ_k for the third adsorption point (see Fig. 1 and text). The vectors $\boldsymbol{\kappa}$ and $\mathbf{e}$ are situated in the YZ plane. The solid line corresponds to $S(\mathbf{k})$ for the fixed azimuthal angle φ_k and the dashed line to $S(\mathbf{k})$ for angle π-φ_k. The angle φ_k is shown in the upper left corner of the figure.

spectra of the molecule N@C$_{60}$ localized on the Si crystal surface.

Figure 3 presents the calculated structural function $S(\mathbf{k})=S(\vartheta_k)$ as a function of the polar angle ϑ_k for the N@C$_{60}$ molecule. Each of these figures corresponds to a fixed azimuthal angle that is within the range $\varphi_k=15°-90°$. The curve corresponding to a fixed azimuthal angle $\varphi_k=0°$ is given in Fig. 2. The calculations show that for a given position of the N@C$_{60}$ molecule on the crystal surface the function $S(\mathbf{k})$ is symmetrical relative to the XZ plane. This symmetry manifests itself in the spectra of photoelectron emission in the *YZ* plane ($\varphi_k=90°$). Owing to this symmetry, the curve corresponding, for example, to an angle $\varphi_k=345°$ coincides exactly with the curve for an angle $\varphi_k=360°-345°=15°$; the spectrum for $\varphi_k=330°$ coincides with the spectrum for an azimuthal angle $\varphi_k=30°$, etc. The set of plots in Fig. 3 gives a full spatial picture of the function $S(\mathbf{k})$ defining the photoelectron angular distribution. It is seen that the three-dimensional (3D) surface described by the structural function is very complicated. According to these figures, the intensity of photoelectron emission rapidly decreases when rotating the plane in which the photoelectrons are recorded. For example, the value of the function $S(\vartheta_k=60°)$ for $\varphi_k=90°$ is only about 6% of the value at $\varphi_k=0°$.

In Fig. 4 the calculated structural function $S(\mathbf{k})$ is plotted for the other point of the molecular adsorption. We consider the case where the molecule as a whole is shifted (without rotation around the *Z* axis) so that the *Z* axis now goes through the middle of the line connecting the Si atoms 1 and 3 in Fig. 1. As before, each of the curves in Fig. 3 represents a polar diagram corresponding to a fixed azimuthal angle that is within the range $\varphi_k=0°-90°$. Because of the absence, in this case, of symmetry in the spectra, the two curves corresponding to the azimuthal angles $\pm\varphi_k$ are given in each of the pictures. These curves are the lines formed by the crossing of the 3D surface of $S(\mathbf{k})$ with a pair of the planes going through the *Z* axis and forming the angles $\pm\varphi_k$ with the *ZX* plane. The difference in the spectra in this figure from those in Fig. 3 is surprising. Their comparison even in one plane of photoelectron emission for $\varphi_k=90°$ allows distinguishing these two points of molecular localization on the (100) surface. The calculations show that nonsymmetry of the surface $S(\mathbf{k})$, relative to the plane the vectors $\mathbf{e}$ and $\boldsymbol{\kappa}$, is a general feature of the spectral behavior when the adsorption point is shifted from point 1 so that the position of the Si atoms is no longer symmetrical relative to this plane.

Consider the next point of molecular localization. Suppose that a projection of the A@C$_{60}$ molecular center onto the (100) plane is along the line 1-8 at a distance $a/4$ from the center atom 1. The calculations show that though the spectra, in this case, are significantly different from the spectra in Fig. 3, they nevertheless remain symmetrical relative to the *XZ* plane since such a position of the molecule in the plane retains the symmetry of the system relative to the plane in which the vectors $\boldsymbol{\kappa}$ and $\mathbf{e}$ are. The situation changes when the vectors are in the *YZ* plane. In this case, because of the absence of symmetry in the positions of the Si atoms relative to this plane, the photoelectron spectra in the planes φ_k and π-φ_k will be asymmetrical, as in Fig. 4. Evolution of the photoelectron spectra, in this case, can be observed in Fig. 5 where the results of the calculations of the structural function $S(\mathbf{k})$ are presented for the case when the photon polarization vector has coordinates $\mathbf{e}(\vartheta_e=60°,\varphi_e=90°)$. Here it is convenient to begin with consideration of the azimuthal angle $\varphi_k=90°$, corresponding to the plane of maximal electron emission, and then investigate the transformation of the spectral shape in the adjacent planes with azimuthal angles φ_k and π-φ_k. The curves in this figure are formed by the crossing of the 3D surface with a pair of the planes going through the *Z* axis and forming equal angles with the *YZ* plane. The difference between the curves in Fig. 5 from those corresponding to other points of molecular adsorption (Figs. 2–4) is so evident that comparison of the spectra even in one plane of photoelectron emission allows distinguishing these three points of molecular localization on the (100) plane.

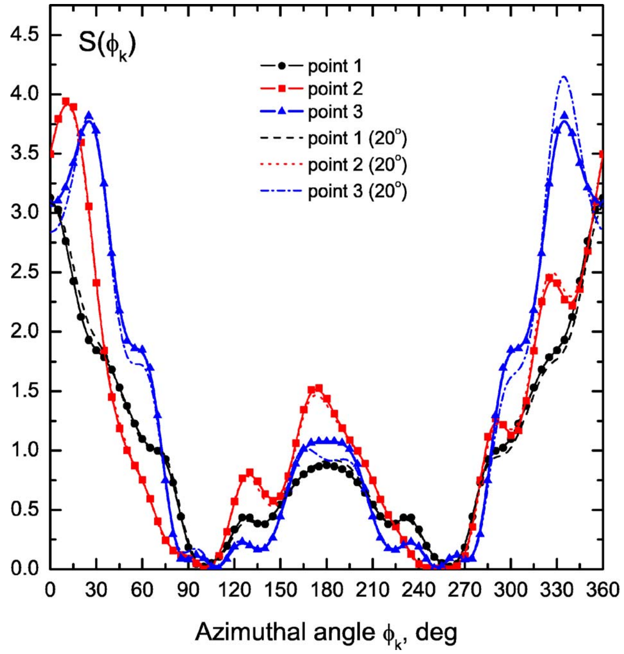

FIG. 6. (Color online) Structural function $S(\mathbf{k})$ as a function of azimuthal angle φ_k at fixed polar angle $\vartheta_k=60°$ for the different adsorption points (see Fig. 1 and text). Dashed, dotted, and dash-dotted curves correspond to the molecule rotated around the *Z* axis as described in the text.

B. Azimuthal dependence of $S(\mathbf{k})$

Consider now the intensity of the beam of electrons with fixed momentum k emitted at a given polar angle ϑ_k, for different azimuthal angles φ_k, measured in an experiment. Such an experiment obtains the curve $S(\mathbf{k})=S(\varphi_k)$ which is a line crossing the surface $S(\mathbf{k})$ and the cone with opening equal to $2\vartheta_k$. A set of such polar diagrams calculated for a set of the polar angles totally defines the shape of the surface $S(\mathbf{k})$. For this calculation we will deal with the case where the wave vector $\boldsymbol{\kappa}$ and the polarization vector $\mathbf{e}$ are in the plane *XZ*, the latter given by spherical angles $\mathbf{e}(\vartheta_e=60°,\varphi_e=0°)$.

In Fig. 6 the azimuthal dependence of the structural functions $S(\mathbf{k})$ as a function of azimuthal angle φ_k is presented for a fixed value of the polar angle $\vartheta_k=60°$ at three points of the N@C$_{60}$ molecule localized on the crystal surface. The choice of the polar angle $\vartheta_k=60°$ is evident—the intensity of photoelectron emission for this angle, as shown by the previous calculations, is maximal. In Fig. 6 it is seen that the intensity of photoemission is maximal in the right semiplane *XZ* ($\varphi_k=0°$) which also contains the vectors $\boldsymbol{\kappa}$ and $\mathbf{e}$. The function $S(\mathbf{k})$ vanishes for azimuthal angles $\varphi_k\approx 90°$ and

270°. The curves corresponding to the first and third points of adsorption are symmetrical relative to the angle $\varphi_k = 180°$ whereas the curve for the second point is visibly asymmetrical. The spectra marked by circles, squares, and triangles correspond to the molecule shifted as a whole without rotation around the Z axis to the first, second, and third points of adsorption, respectively. In the same figure the calculated results of the function $S(\mathbf{k})$ are presented for the molecule located at these points but rotated around the normal to the surface (the Z axis) to the angle 20° counterclockwise, looking at the surface from point A. It is interesting to note that under such a rotation the spectrum corresponding to the third point is subject to maximal deformation while the originally asymmetrical curve $S(\varphi_k)$ for the second point of adsorption is changed comparatively only weakly.

V. CONCLUSIONS

In this paper, we have considered two possible schemes for determining the position of a $N@C_{60}$ molecule adsorbed on a Si (100) surface by measuring the angular distribution of electrons photoejected from the 1s level of the encapsulated N atom. The first involves the study of the structural function $S(\mathbf{k})$ as a function of the polar angle ϑ_k for fixed electron momentum k and azimuthal angle φ_k. The second investigates the dependence of $S(\mathbf{k})$ on the azimuthal angle. In both cases it has been established that the polar angle and azimuthal angle dependence of the shape of the photoelectron angular distribution is extremely sensitive to both the location of the molecule on the surface of the Si and the orientation of the molecular axis of the fullerene cage relative to the crystallographic directions. This finding can, in principle, be used for the diagnostics of molecular localization on the surface. We believe that the results of this calculation will stimulate and, to some extent, direct experimental studies in this rapidly developing field of photoelectron spectroscopy and nanotechnology.

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