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Carbon *KVV* Auger line shapes of graphite and stage-one cesium and lithium intercalated graphite

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A symmetry-resolved one-electron density of states (DOS) for graphite is extracted from existent x-ray photoelectron and x-ray emission spectroscopy (XES) data and used in conjunction with empirical atomic matrix elements to construct a carbon *KVV* Auger line shape for graphite which is in substantial agreement with experiment. For the intercalated graphites, an additional peak is added to the graphite one-electron DOS near the Fermi energy. In the absence of available XES data for C_8Cs and C_6Li, the energy and intensity of this peak are determined by fitting the C *KVV* Auger spectra. The enhanced intensities found for this peak, relative to the ultraviolet photoelectron spectroscopy data, are interpreted as being due to the screening charge surrounding the C 1*s* core. The measure of this enhancement corresponds to 0.5 and 0.6 electrons (intercalant charge donation plus screening) on the core-ionized carbon atom for the case of C_8Cs and C_6Li, respectively. No evidence is found for the selection rule or large matrix-element effects postulated in previous work.

I. INTRODUCTION

Graphite intercalation compounds have been the subject of considerable attention because of their novel electronic and structural properties.[1–5] Electron spectroscopies have been used to probe the band-structure and electron densities of states for both graphite and the various intercalation compounds. Photoemission,[6–8] electron loss,[9,10] and Auger electron spectroscopic[11] work has been reported.

Recent band-structure calculations have been done on C_6Li, [12,13] C_8K,[14–17] acceptor compounds,[18] and higher stage compounds.[19] The results for the alkali graphite intercalation compounds (AGIC) show enhanced density of states at the Fermi level, as argued by Spain and Nagel[5] on simple physical concepts. Fractional charge is transferred from the alkali into the graphite conduction band. Evidence for the charge transfer can be inferred from NMR chemical shifts (C_8Cs),[20] Mossbauer (C_8Cs),[21] and core-level x-ray photoelectron spectroscopy (XPS) chemical shifts (C_6Li, C_8Rb).[7] Changes in the valence-band photoemission intensities due to intercalation[6–8] are also evident, however, photoemission does not provide direct information on any localization of the occupied electron wave functions. Because of the core state involved in x-ray emission (XES) and Auger electron (AES) spectroscopies, they are sensitive to the electron wave functions localized about that core hole and can be used to directly examine charge transfer. No XES data have been reported for AGIC, but AES data on alkali-metal intercalated graphite have recently been published by Oelhafen and co-workers.[11] In some very nice work they show by ultraviolet photoelectron spectroscopy (UPS) that the AGIC have a narrow peak in the density of states (DOS) at the Fermi level and that this peak is also reflected in the carbon Auger spectrum. In their interpretation of the data they concluded that the peak in the one-electron DOS at the Fermi level is mainly due to alkali states and that because of matrix-element effects, these states are not significantly convoluted with the rest of the band C *KVV* Auger transition.

For the kinetic energy of the carbon Auger, the probability for interatomic (i.e., two-center) Auger transitions is substantially smaller than for intra-atomic (one-center) transitions.[22] Thus the strong presence of the well-defined sharp peak at the high kinetic-energy side of the carbon Auger line shape is more likely due to charge transferred from the alkali into the carbon π electron conduction band. Bader[23] has performed a more thorough theoretical examination of the AGIC Auger line shape. He finds no evidence that the high-kinetic-energy alkali-induced feature is not convoluted with the rest of the graphite valence band, a conclusion with which we agree. However, he had to invoke strong matrix-element effects in his analysis. On a per electron basis, he requires π electrons to contribute three times as much as σ electrons to the Auger line shape in both graphite and AGIC. We disagree with this as it shifts the principal peak in the Auger spectrum of graphite to too high a kinetic energy.

The interpretation of Auger line shapes is not simple. In order to have confidence in the interpretation of the C_{AES} in AGIC, we first address graphite. The graphite C_{AES} has been published by three groups.[24–26] Each group corrected the raw data for baseline and electron-loss features, calculated the transition density of states as proposed by Lander (by self-deconvolution),[27] and compared the results with XPS, XES, and theoretical measures of the electron density of states. General agreement is found for the positions of the peaks in the valence band. Careful comparison of intensities was not attempted because the transition density of states contains both density of states and matrix-element contributions. Since we wish to compare critically intensities, rather than take a self-deconvolution of the experimental Auger, in Sec. II we will calculate the Auger line shape via the techniques of Ramaker and Murday.[28–32] The one-electron density of states is deduced from XPS[33–35] and XES[36–38] spectra and compared with the theoretical[39] density of states (DOS). The Auger line shape is calculated by convolving the one-electron bands, weighted by appropriate matrix elements. This approach provides a theoretical spectrum which compares well with the experimental data of Levenson.[26]

The AGIC Auger Line shapes are examined in Sec. III. An additional narrow band in the one-electron DOS is added at the Fermi level. This band is made to fit the AES data of Oelhafen[11] and then used to calculate the one-electron DOS. The general features of the experimental UPS line shape are reproduced, but the one-electron intensity of the low-binding -energy additional peak is very large. Some reasons for this, i.e., AES initial-state screening and matrix-element effects, are discussed. There is no evidence that the Fermi-level peak is not convolved with the rest of the graphite band.

II. C AUGER LINE SHAPE IN GRAPHITE

For systems in which the final-state hole-hole correlation energy is smaller than the appropriate bandwidth, it has been shown that the Auger line shapes reflect the one-electron density of states[32,40,41] modified by matrix-element effects[42] and screening.[43] A one-electron density of states in carbon can be determined from $K\alpha$—x-ray emission and valence-band x-ray photoemission data. Because of the dipole selection rules, the $K\alpha$—XES data show only the $2p$ electron density of states; the XPS matrix-element selects primarily the $2s$ density of states.[44] There have been several measurements of the $K\alpha$ line shapes for graphite which all show the same general features, but with varying intensities, especially at the higher energies.[36–38] The polarized emission study of Beyreuther and Wiech[38] shows that this variation is likely due to angular dependences in the K emission. Since the σ orbitals extend mainly perpendicular to the c axis, the $\sigma \rightarrow 1s$ radiation is polarized perpendicular to that axis; similarly the $\pi \rightarrow 1s$ transition is polarized parallel to the c axis. In Beyreuther and Wiech, the XES line shape at 80° take-off angle is attributed to essentially pure σ band modified by any transition-probability matrix elements and the Auger effect. We take that measured line shape to be pure σ_p density of states. The π_p line shape is calculated from the 5° take-off angle data by assuming its 275.5 eV peak is a pure σ_p and subtracting out a normalized 80° take-off line shape. The area under the σ_p line shape is then normalized to twice the area under the π_p line shape; this normalization presumes pure sp^2 bonding in the σ bands and a single p electron in the π band. It should be noted that the XES and AES both sample the electron wave functions local to the initial core hole. If there are substantial matrix-element distortions across the band due to band-induced variation in the local density,[45] then this method of deducing the one-electron density of states for use in the Auger line-shape calculation has a first-order correction for those distortions.

McFeely *et al.*[34] point out that their x-ray photoemission study of the graphite valence band has a cross-section ratio of $\sigma(2s)/\sigma(2p) \simeq 13$. The Scofield[44] cross sections for Al $K\alpha$ give a ratio of $\sigma(2s)/\sigma(2p) \approx 10.6$. From the McFeely *et al.* measurement (which is corrected for the inelastic loss contributions and includes an extrapolated cut off at the bottom of the band to eliminate artificial tailing), we calculate the σ_s line shape by requiring the XPS line shape to be the sum of $\sigma_s + \frac{1}{32}(\sigma_p + \pi_p)$. (The XES and XPS energy scales are reconciled by subtracting from the XES data the energy of the carbon 1*s* core hole, which is taken to be 284.5 eV.[34,35] Here and throughout this work our resolution in digitizing published experimental data is approximately 0.5 eV.) The area under the σ_s line shape is then normalized to be one half of the σ_p line shape area as required by a pure sp^2 band.

In Fig. 1 we present the experimentally derived line shape in both its localized (appropriate to XES and AES) and delocalized (appropriate to photoemission) form. The difference between localized and delocalized arises from consideration of the normalization of the Bloch eigenfunctions [Ref. 45(a), Eq. (1)]. We treat this effect approximately by considering only nearest-neighbor overlap integrals of Slater-type orbitals optimized for the carbon atom[46] and linearly interpolating the respective normalization factors between the top and bottom of the σ band and the π band. This effect is quite small and both line shapes agree fairly well with the theoretical line shape of Painter *et al.*,[39] Gaussian broadened by 2 eV to account for the several sources of line broadening. The agreement in the deep-valence region, i.e., high-binding energy, would be improved if we had included an energy dependence into the broadening function to account for Auger decay in the valence band which is energy forbidden in the shallow valence region.[47] Furthermore, this agreement between experiment and theory suggests that matrix-element effects in XES (and by extrapolation AES) are not very large.

We assume that atomic neon *KVV* Auger matrix elements[48] are valid for graphite. The graphite intensities are then simply related to the neon *KVV* intensities by the ratio of available valence electrons between the Ne and graphite. This approximation has proven successful for oxygen and nitrogen containing compounds.[31,32] The per electron

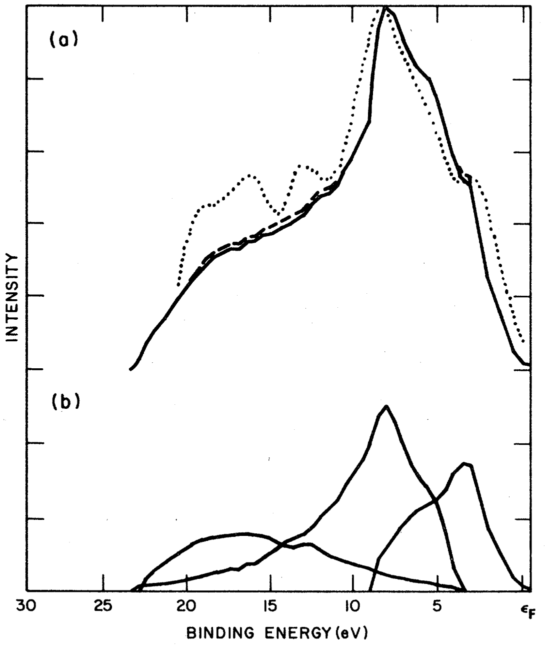

FIG. 1. (a) The occupied DOS for graphite from band-structure calculations (Ref. 39) (· · · ·), from XES and XPS data (——), and in local form appropriate to XES and AES (— — —). The intensities are normalized to their peak values. (b) The decomposition of the local DOS for graphite. In order of increasing binding energy are the bonding π band, the *p* component of the σ band, and the *s* component of the σ band.

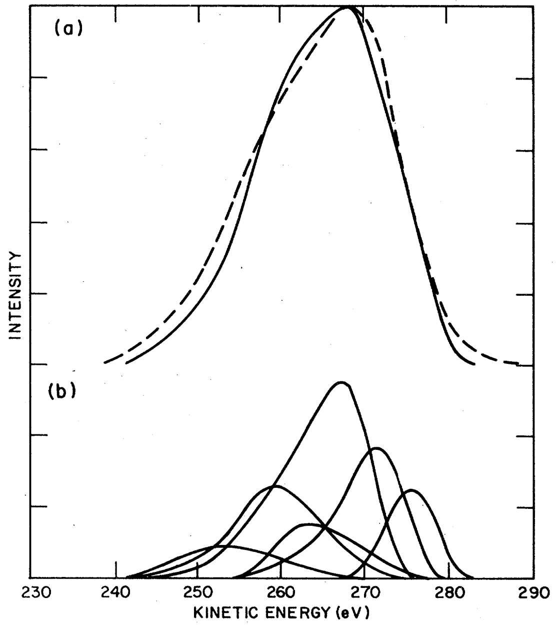

FIG. 2. (a) The C *KVV* Auger line shapes of graphite: experimental (Ref. 26) (— — —) adjusted by 5 eV to correct for the work function and our theoretical result (——). The intensities are normalized to their peak values. (b) The decomposition of our theoretical line shape. The contributions, in order of increasing kinetic energy, are $\sigma_s\sigma_s$, $\sigma_s\sigma_p$, $\sigma_s\pi$, $\sigma_p\sigma_p$, $\sigma_p\pi$, and $\pi\pi$.

matrix elements that we use, normalized to *pp*, are $pp = 1.0$, $sp = 1.0$, and $ss = 0.8$. The C Auger line shape for graphite is readily calculated by convolving the line shapes, multiplying them by the appropriate matrix element, and taking the sum. The absolute energy is fixed by taking the C_{1s} binding energy as 284.5 ev.[34,35] The calculated Auger line shape is compared with the Smith[26] line shape in Fig. 2(a); the contributions to the line shape from the various parts of the valence bands are illustrated in Fig. 2(b). The general features are reproduced quite well. Some discrepancies exist on both the high- and low-energy wings. These may be due to problems in the experimental data reduction[25,49] or to some of the simplifications inherent in our theoretical techniques. In particular, the agreement on the low-energy wing must be considered somewhat fortuitous due to uncertainties in data reduction. The high-energy side of the line shape is more certain experimentally because the base line extrapolation is less and the inelastic-loss correction is reduced.

Note that had we assumed matrix-element effects and made the π-π contribution [the highest kinetic-energy peak in the decomposition of our constructed line shape, Fig. 2(b)] dominate the Auger line shape,[23] our line shape would have had its maximum at 275 eV rather than the 268 eV which agrees with experiment to within an electron volt.

III. C AUGER LINE SHAPE IN AGIC

The UPS data from the AGIC show that the intercalant creates a peak in the density of states at the Fermi level and that to a first approximation the graphite features are simply shifted slightly to higher-binding energies by 1 eV,[6] consistent with the rigid-band model. Thus, in order to treat the AGIC's we simply shift our experimentally derived graphite density of states 1 eV to higher-binding energy (relative to ϵ_F) and add a single new peak. The functional form of this new peak and its location in energy relative to the graphite DOS is adjusted to reproduce the observed Auger line shapes. The one-electron energies deduced from this fit are referenced to the Fermi level by subtracting a C_{1s} binding energy of 285 eV.[6,35]

The calculated Auger line shapes for C_8Cs and C_6Li samples are compared with the measured line shapes in Figs. 3(a) and 4(a), respectively. The various contributions to the total Auger line shape are shown in Figs. 3(b) and 4(b); the cross terms between the three graphite contributions and the intercalant contribution are present and are necessary for the theory to reproduce the data. For both C_6Li and C_8K there is some unaccounted experimental intensity in the cross-fold region, and the peak of the theoretical line shape is at ~ 1 eV lower kinetic energy. Both of these small differences disappear if the graphite DOS is shifted down in energy by only 0.5 eV rather than 1.0 eV. The present excess of experimental intensity in the cross-fold region provides no reason to postulate diminished matrix elements for the cross terms.

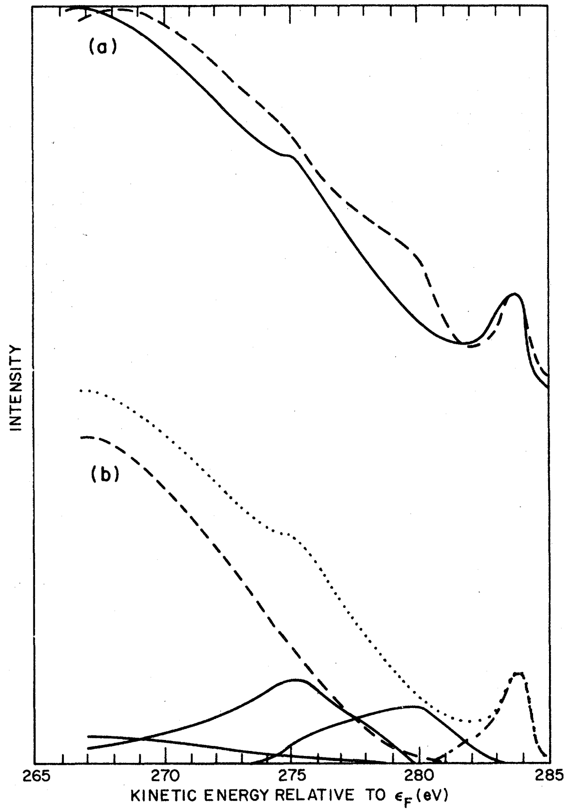

FIG. 3. (a) The experimental (Ref. 11) (— — —) and theoretical (——) C *KVV* Auger line shapes of C_8Cs. The intensities are normalized to their peak values. The experimental peak has not been corrected for electron-loss contributions. (b) The decomposition of the theoretical carbon Auger line shape (· · · ·) into its graphite component (— — —), the self-fold of the Cs donated DOS (—·—), and the cross folds of the Cs donated DOS with the σ_s, σ_p, and π bands (——) in order of increasing kinetic energy. Note the substantial intensity in the region 275 to 280 eV resulting from those cross folds.

In Fig. 5 the low-binding-energy portion of our one-electron DOS, used to construct the Auger line

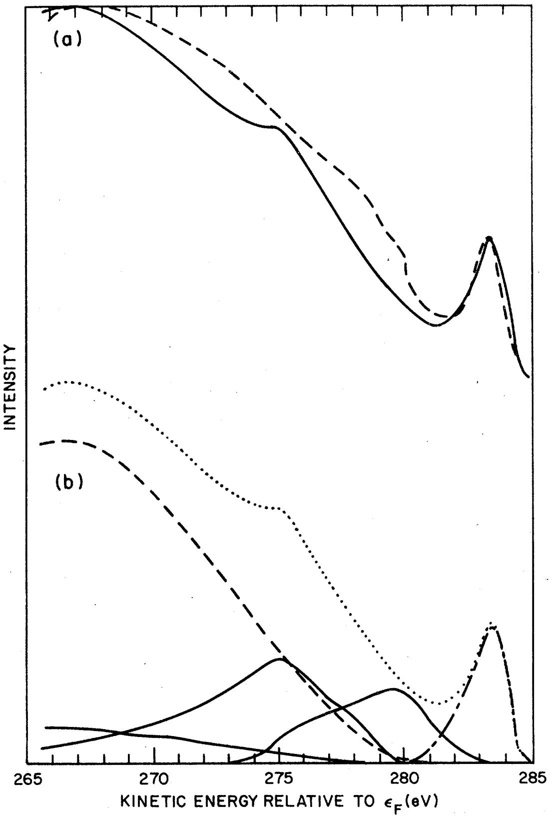

FIG. 4. (a) The experimental (Ref. 11) (— — —) and theoretical (——) C *KVV* Auger line shapes of C_6Li. The intensities are normalized to their peak values. (b) The decomposition of the theoretical carbon Auger line shape (· · · ·) into its graphite component (— — —), the self-fold of the Li donated DOS (—·—), and the cross folds of the Li donated DOS with the σ_s, σ_p, and π bands (——) in order of increasing kinetic energy. Note the substantial intensity of the region 275 to 280 eV resulting from those cross folds.

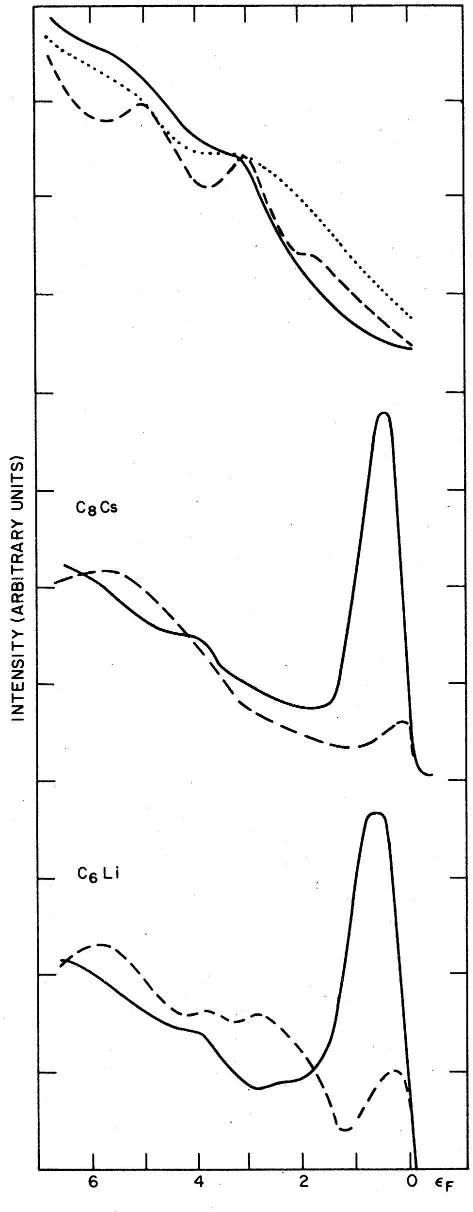

FIG. 5. One-electron DOS for graphite and stage-one cesium and lithium intercalated graphite. The normalizations of the various curves are not simply related. Top: DOS for graphite from band-structure calculations (Ref. 39) (· · ·), from UPS (Ref. 6) (— — —), and from XES/XPS (——). Middle: The DOS for C_8Cs from UPS (Ref. 6) (— — —) and that constructed by shifting the graphite local XES/XPS curve 1 eV higher in binding energy and adding a peak near the Fermi energy. The intensity and energy of the new peak is determined by fitting the Auger spectra (——). Bottom: DOS for C_6Li from UPS (— — —) and our construction as described above (——).

shape for graphite, is compared with UPS and theory. Also in the same figure we compare our one-electron DOS for C_8Cs and C_6Li with UPS data. Owing to base line effects in UPS, which have not been substracted, the intensities have been normalized somewhat arbitrarily. However, for the AGIC there is a significant discrepancy between the one-electron intensity for the intercalant peak deduced by fitting the Auger data compared with the one-electron DOS from the UPS measurements. The AES line shape requires far greater electron density in the intercalant peak than does the UPS. The UPS intensity is proportional to

$$\alpha[N_\pi^G(E)+N_\pi^T(E)]+N_{2S}^A(E)$$

where $N_\pi^G(E)$ is the electron density in the normal graphite π band, $N_{\pi}^{T}(E)$ is the electron density donated into the π band by the alkali, $N_{2s}^{A}(E)$ is the electron density local to the alkali, and α is a scale factor to account for UPS matrix elements. Since the Auger process is local, C_{AES} samples primarily the N_{π}^{G} and N_{π}^{T} electron densities. The UPS spectra must add a N_{2s}^{A} contribution and should have the larger peak intensity. One might argue that matrix-element effects in the Auger process effectively increase N_{π}^{T} relative to N_{π}^{G}. However, these two densities are, to good approximation, the bonding π and antibonding π^* bands of graphite. In our treatment of the Auger line shape of graphite we found no evidence for significant differences in Auger matrix elements involving the bonding π band relative to the σ band. Thus, it is unlikely that π-π^* matrix-element effects are responsible for this discrepency.

A second possible cause for the apparent discrepancy is screening. The UPS measurement has a filled initial state and a single-hole final state. The Auger transition has an initial screened-core-hole, and a two-hole final state. The screening charge for the initial core hole will come at the Fermi level and augment the N_{π} population. The ratios of the area of the intercalant peak to the area of the graphite π band are 0.6 for C_6Li, and 0.5 for C_8Cs. If this were an accurate measure of the ground-state charge transfer, it would correspond to a transfer of ~ 4 electrons in each case from the alkali donor. Since one electron is the maximal transfer, screening of the initial-state core hole must substantially augment the local π charge. There is some uncertainty in the sensitivity of AES line shapes to screening charge. Even if a significant portion of the screening charge surrounding a C 1*s* core hole in the AGIC's resides on that atom, a theoretical result[50] indicates that it would not be seen in XES and by implication AES. This conclusion conflicts with a more recent experimental and theoretical study of the Auger spectrum of Be.[43] An experimental study of screening in AES for simple metals is not conclusive.[51] This graphite data show strong evidence for screening effects in the AES.

IV. CONCLUSIONS

We have derived a symmetry resolved density of states for graphite from existent XPS and XES data which is in substantial agreement with theory.[39] Using this DOS together with atomic Auger matrix elements, we have generated a graphite C *KVV* Auger line shape which is in substantial agreement with experiment. In contrast with the work of Bader[23] we do not need to hypothesize large Auger matrix-element effects, which are not justified by simple consideration of the normalization of the Block wave functions for graphite,[45] in order to attain this agreement.

For the case of C_8Cs and C_6Li AGIC's XES data are not available and, using in its place UPS data, this methodology does not work. Both the AES and UPS deduced versions of the one-electron DOS have a new peak slightly below the Fermi level. A slight downward shift in the energy of the AES-deduced peak compared to the UPS data is on the order of the resolution used in digitizing the various experimental data. However to fit the AES, we must drastically increase the intensity of the peak at the Fermi level for both C_8Cs and C_6Li. We attribute the significant intensity change to the screening of the initial-state core hole of the Auger process and consequently, predict that XES spectra of AGIC's would show similar enhancements of the peak at the Fermi level. Assuming that in the absence of a core hole the alkali atom donates the maximum (one electron) to the antibonding π band of graphite, the additional measure of this peak would indicate that, of the screening charge around a 1*s* carbon core hole, 0.4 (0.5) of an electron resides on the atom having that core hole in C_8Cs (C_6Li). Perhaps, the Thomas-Fermi model can be used to substantiate this finding.[52,53]

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