Positron energy levels in semiconductors

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Positron affinities, deformation potentials, and lifetimes are calculated in diamond, Si, SiC, and BN bulk cubic semiconductors using the first principles pseudopotential and linear-muffin-tin-orbital (LMTO) methods. Both the electron and positron energies are calculated within the local density approximation and generalized gradient approximation (GGA). It is observed that the LMTO calculated values of quantities of interest are systematically lower than those calculated with the pseudopotential method. Results further show that the GGA correction for the electron energy levels is not very important in positron calculations. The calculated positron affinity in SiC is found to be in reasonable agreement with experiment. Positron properties for other materials are also compared with available experimental data.

I. INTRODUCTION

Positron energy levels in solids are quite difficult to examine experimentally. In semiconductors the interpretation of experiments is further complicated by surface effects. From the theoretical point of view ordinary techniques to examine the electronic structure of (periodic) solids cannot handle such effects. Fortunately, the sum of electron and positron chemical potentials is independent of the surface properties, and standard computational electronic structure methods can be used to calculate it. This sum, usually called the positron affinity, can also be obtained experimentally via work function measurements.

The electron work function in a solid is defined as the minimum energy needed to take an electron from the Fermi level deep within the bulk region to the vacuum.[1] In order to separate the bulk and surface contributions, the electron work function is usually expressed as $\phi_- = -\mu_- + \Delta$ where μ_- is the bulk chemical potential and Δ is the surface dipole potential arising from the surface structure and surface chemistry. The positron work function is defined as the minimum energy gained to bring a thermalized positron from the vacuum into the lowest bulk energy level, which is identified with the positron chemical potential μ_+. In terms of the separation into bulk and surface contributions, the positron work function is expressed as $\phi_+ = -\mu_+ - \Delta$. Due to the large surface dipole potential, the positron is seen to be emitted in most solids. In semiconductors there is band bending near the surface due to surface charge density.[2] As a result of this both the electron and positron work functions are modified by the corresponding electric field arising from the surface band bending, i.e., $\phi_\mp = -\mu_\mp \pm \Delta \pm E_s$, where E_s is the energy required to produce the electric field.

The positron affinity in semiconductors can be viewed in two different ways. First, it can be defined as the energy gained by taking a thermalized positron from the vacuum to the lowest bulk energy level close to the surface.[2] Due to the surface band bending the positron affinity (designated in this case usually as χ_+) is different from the positron work func-

tion in semiconductors, whereas in metals the positron affinity is the same as the positron work function. The electron affinity (χ_-) does not change due to surface band bending.[2]

The other definition of the positron affinity (labeled often as A_+) by Puska *et al.*[3] is related to the positron absolute energy levels in different materials. That is, the positron affinity is introduced through $A_+ = \mu_- + \mu_+$ and is thus a pure bulk property of the material. This definition can also be expressed as $A_+ = -(\phi_- + \phi_+)$. Since Δ and E_s have contributions to the electron and positron work functions, equal in magnitude and opposite in sign, they cancel out in the sum, leaving μ_- and μ_+ only. This second notion of the positron affinity (A_+) is used in the present paper. Such a positron affinity is examined with a good precision in the positron emission spectroscopy method.[4,5]

Positrons implanted into a solid start to diffuse after their thermalization owing to positron-phonon interactions. The positron diffusion in a semiconductor at low temperatures is dominated by a free positron interacting with longitudinal acoustic phonons. In the deformation potential theory the positron diffusion constant D_+ due to the acoustic phonon scattering is given by[6]

$$D_+ = \left(\frac{8\pi}{9}\right)^{1/2} \frac{\hbar^4 c_L}{(m_+^*)^{5/2}(k_B T)^{1/2} E_d^2}, \qquad (1)$$

where E_d is the positron deformation potential, m_+^* is the positron effective mass, T is the absolute temperature, and c_L is the elastic constant associated with the longitudinal waves averaged over the directions of propagation.

The conventional method for calculating the positron affinity is based on density functional theory where the electron and positron energy levels are calculated with respect to the common reference level called the crystal zero of the infinite lattice.[7] The method of choosing the crystal zero is completely dependent on the electronic structure scheme taken for calculating the energy band structure of the solid. For example, in the linear-muffin-tin-orbital method within the atomic sphere approximation[3,8] (LMTO-ASA) the Cou-

lomb potential on the surface of the Wigner-Seitz sphere is taken as the crystal zero, and in the augmented plane wave method the average of the Coulomb potential between the muffin-tin sphere and the Wigner-Seitz cell is taken as the crystal zero.[9] In bulk positron affinity calculations explicit determination of the crystal zero level is not needed, as its particular values for electrons and positrons have the same magnitude and opposite sign in the electron and positron chemical potential calculations.

In the present work we have used the first principles pseudopotential method for calculating positron affinities. The advantage of this method is that it can be used to calculate affinities and deformation potentials in semiconductors with defects where the lattice relaxations at the defect site play an important role in changing the electron and positron energy levels.[1] The LMTO-ASA technique has also been employed for comparison.

As for the materials studied, we have chosen the following cubic semiconductors: diamond, silicon, silicon carbide (SiC), and boron nitride (BN). The purpose of the present paper is to compare theoretical results obtained with available experimental findings. Recently, positron affinities have been studied experimentally in diamond[2] and both experimental and theoretical studies have been undertaken for several structural modifications of SiC.[10,11] Regarding Si, it is expected[12] that it has a negative positron work function like diamond and SiC. Boron nitride has not yet been investigated from the point of view of positron work function and affinity and we give here a prediction of its properties.

The paper is organized as follows. In Sec. II we explain briefly the theoretical background for electronic structure calculations and determination of positron levels in the materials studied. Section III deals with results and their discussion. The paper is concluded in Sec. IV.

II. METHODS FOR ELECTRONIC STRUCTURE AND POSITRON STATE CALCULATIONS

The details of positron affinity and deformation potential calculations using the first principles pseudopotential technique have been described in our earlier work.[13] Here only the essential features of the method will be described. Norm conserving pseudopotentials of Bachelet-Hamann-Schlüter type[14] are used to calculate electronic structure in semiconductors. The electron chemical potential in this method is calculated as $\mu_- = E_v + \alpha + V_0$, where E_v is the top of the valence band, α is the pseudocore correction, and V_0 is the average Coulomb potential in the solid. The quantity α corrects the pseudo nature of the electron ion-core potential. After this correction the ion-core potential is a point-core potential which does not include any contribution from the core orbitals.[15] In order to calculate the positron affinity in a solid, the positron states need to be calculated with the same electron Coulomb potential but with opposite sign to maintain the same V_0 in both calculations. Therefore the positron ion-core potential is constructed in the point-core approximation. The positron chemical potential is thus expressed as $\mu_+ = E_0 - V_0$, where E_0 is the ground state energy including positron correlation energy.

Determination of the electron and positron chemical potentials needs the calculation of the average Coulomb poten-

tial (V_0) in the bulk solid. However, the average potential in an infinite solid without a surface is not uniquely defined.[16] Since the contribution of V_0 is equal and opposite in μ_- and μ_+, it is canceled in the final expression for A_+,

$$A_+ = E_v + E_0 + \alpha. \tag{2}$$

The positron deformation potential (E_d) is obtained from the volume derivative of the positron affinity using the expression[1]

$$E_d = \Omega \frac{\partial A_+}{\partial \Omega}, \tag{3}$$

where Ω is the volume of the crystal.

The bulk positron lifetime τ is another valuable quantity to check the correctness of the density functional calculations. It is the inverse of the annihilation rate[1]

$$\lambda = \tau^{-1} = \pi r_0^2 c \int n(\mathbf{r}) n_+(\mathbf{r}) \gamma(\mathbf{r}) \, d\mathbf{r}, \tag{4}$$

where $n(\mathbf{r})$ is the total electron charge density, $n_+(\mathbf{r})$ stands for the positron density, and $\gamma(\mathbf{r})$ denotes the enhancement factor. Furthermore, r_0 is the classical electron radius and c is the speed of light.

Concerning core electrons, which essentially do not enter the pseudopontential calculations, Louie et al.[17] have shown that their inclusion into the exchange-correlation potential indirectly by the nonlinear core correction (NLCC) method reproduces structural properties of the solids which can be compared with those obtained from all-electron methods. We use the NLCC technique in our pseudopotential calculations. The band structure calculation has been carried out in the momentum space method with a plane wave basis set.[15] The charge density is evaluated by performing Brillouin zone summation in the Chadi-Cohen two-point scheme.[18]

For the sake of comparison, we have also employed the LMTO-ASA method already mentioned above and computed all positron quantities of interest. Details of our calculations are presented in Refs. 10 and 11. We just note here that we have incorporated appropriate empty spheres into crystal structures to better describe the interstitial charge distribution. Into the basis we have included s, p, and d orbitals, treating d orbitals as downfolded.[8]

For the electron exchange-correlation potential we have utilized two approaches. The first is the local density approximation (LDA). In this case, we take the scheme of Ceperley and Alder[19] as parametrized by Perdew and Zunger.[20] Furthermore, the ground state properties of solids seem to be reproduced well by incorporating inhomogeneity effects in the energy functional within the generalized gradient approximation[21–25] (GGA). The Perdew-Wang GGA scheme[22] has been used here. The GGA potentials in momentum space (needed in pseudopotential calculations) are evaluated by the method prescribed by White and Bird.[26]

Barbiellini et al.[27,28] have shown that the inclusion of a gradient correction in the positron correlation term reproduces the experimental lifetimes of metals, semiconductors, and insulators. In addition to that, the positron affinities in some metals calculated in this scheme agree quite well with

TABLE I. Structural data for semiconductors studied: lattice constant (a_0), structure type, and space group.

	a_0 (Å)	Structure type	Space group
Diamond	3.58	diamond	$Fd3m$
Si	5.43	diamond	$Fd3m$
SiC	4.35	zinc blende	$F43m$
BN	3.62	zinc blende	$F43m$

experiment. Finally, in LDA positron calculations the form of the positron correlation potential from Ref. 29 has been taken.

III. RESULTS AND DISCUSSION

Lattice constants for all systems studied are specified in Table I together with other structural data. The positron affinities, deformation potentials, and lifetimes are calculated first using the positron LDA formalism.[29] The enhancement factor [see Eq. (4)] is taken from Ref. 30. The results obtained using the pseudopotential and LMTO-ASA methods are presented in Tables II and III, respectively. The tables contain results of calculations for both electron LDA and GGA. Analogously, Tables IV and V show results of calculations obtained using the positron GGA formalism.[27] In this case the enhancement factor from Ref. 27 is employed.

From the results presented it is clear that the treatment of the electron exchange-correlation potential in the GGA method does not have any significant effect on the calculated affinities, deformation potentials, and lifetimes when compared with the LDA results. It is also clear that the GGA scheme had no effect on the calculated positron angular correlation in Si (Ref. 31) as the positron avoids the ion-core region where the gradient of the electron density is high. The difference between the GGA and LDA approaches would probably be more apparent if optimization of the lattice constants with respect to the total energy were performed before calculating the positron properties.

Concerning the difference between the LDA and GGA schemes for positrons, the positron affinities are shifted up (their magnitudes are reduced) in the case of the GGA due to the GGA correction in the positron correlation energy, which leads to a more repulsive positron potential compared to the LDA. To be precise, the GGA scheme results in several tenths of eV shift of A_+ values with respect to the LDA

TABLE III. Positron properties in semiconductors calculated using the LMTO-ASA method and Boroński-Nieminen LDA formalism (Ref. 29). The meaning of the symbols is the same as in Table II.

	LDA			GGA		
	A_+ (eV)	E_d (eV)	τ (ps)	A_+ (eV)	E_d (eV)	τ (ps)
Diamond	−3.02	−13.24	94	−2.80	−13.26	94
Si	−7.17	−6.15	214	−7.01	−6.20	214
SiC	−5.51	−8.07	137	−5.33	−8.11	137
BN	−4.57	−11.38	98	−4.34	−11.39	99

calculation, which was also observed in the case of metals in Ref. 27. A similar effect occurs for the deformation potentials (except for Si calculated with the pseudopotential method) even if the shift is not so large as for affinities. No systematic trend can be observed for lifetimes.

The comparison of results calculated using the pseudopotential and LMTO-ASA techniques is as follows. The LMTO-ASA positron affinities are systematically lower than the pseudopotential ones. The same conclusion holds for positron lifetimes in accordance with calculations of Rojas *et al.*,[32] where the LDA scheme for positrons was applied to several elemental semiconductors. With the exception of Si and SiC the deformation potentials are also shifted down. The origin of these systematic shifts might be in the atomic sphere approximation[8] and in the fact that the description of interstitial electron and positron charge distributions may not be fully realistic even if empty spheres have been included into the crystal lattice of the semiconductors studied (see Sec. II). On the other hand, the pseudopotential technique also incorporates several approximations (see Sec. II). To clarify the adequacy of both computational techniques used, a full potential calculation including core electrons (i.e., an all-electron calculation) is required.

From Tables II–V it is clear that the lifetimes, affinities, and deformation potentials for different semiconductors are correlated mainly with their lattice constants (see Table I). Siethoff[33] has shown that the bulk lifetime is proportional to $a_0^{3/2}$ with a_0 being the lattice constant. We have checked if the affinities and deformation potentials in semiconductors can be scaled with the lattice constant. For this purpose we consider the results obtained using the LDA approach for

TABLE II. Theoretical positron affinities (A_+), deformation potentials (E_d), and lifetimes (τ) in semiconductors calculated using the pseudopotential technique. The positron correlation energy is considered in the Boroński-Nieminen LDA formalism (Ref. 29). Both LDA and GGA approaches for electrons are used.

	LDA			GGA		
	A_+ (eV)	E_d (eV)	τ (ps)	A_+ (eV)	E_d (eV)	τ (ps)
Diamond	−2.64	−12.01	100	−2.64	−11.92	99
Si	−6.48	−6.48	217	−6.45	−6.39	217
SiC	−4.58	−8.76	145	−4.42	−8.73	145
BN	−3.91	−10.62	102	−4.10	−10.63	102

TABLE IV. Theoretical positron affinities (A_+), deformation potentials (E_d), and lifetimes (τ) in semiconductors calculated using the pseudopotential technique. The positron correlation energy is considered in the GGA formalism by Barbiellini *et al.* (Ref. 27). Both LDA and GGA approaches for electrons are used.

	LDA			GGA		
	A_+ (eV)	E_d (eV)	τ (ps)	A_+ (eV)	E_d (eV)	τ (ps)
Diamond	−2.24	−11.79	100	−2.20	−11.67	100
Si	−5.98	−6.51	215	−5.91	−6.41	216
SiC	−4.10	−8.60	143	−3.92	−8.55	144
BN	−3.37	−10.60	105	−3.15	−10.57	105

TABLE V. Positron properties in semiconductors calculated using the LMTO-ASA method and Barbiellini *et al.* GGA formalism. (Ref. 27). See Table IV for explanation of symbols.

	LDA			GGA		
	A_+ (eV)	E_d (eV)	τ (ps)	A_+ (eV)	E_d (eV)	τ (ps)
Diamond	-2.42	-13.09	98	-2.17	-13.10	99
Si	-6.74	-5.94	211	-6.57	-5.97	211
SiC	-5.05	-7.97	138	-4.85	-7.99	138
BN	-3.94	-11.30	104	-3.70	-11.30	105

both electrons and positrons (Tables II and III). No such scaling is possible for the affinity data. Concerning the pseudopotential results the deformation potential can be scaled as $E_d = -C/a_0^{3/2}$, where $C = -81$ eV Å$^{3/2}$ for diamond, Si, and SiC (see Fig. 1, solid line). However, it is surprising to find that boron nitride does not fit into this line. We have no physical reason for this behavior at present, but it is quite common that semiconductors consisting of nitrogen (among other elements) behave differently.[25] Fitting the LMTO-ASA results in the same way (see Fig. 1, dotted line) gives $C = -83$ eV Å$^{3/2}$, but the calculated points exhibit rather large scatter with respect to the fitted line. This further indicates that the above scaling relation is only approximate.

Let us now discuss our results for particular systems in more detail.

A. Diamond

Li *et al.*[34] have measured the positron lifetime in diamond to be 97.5 ± 1.5 ps. From Tables II–V it is found that the lifetime calculated by treating the V_{xc} and V_{corr} in the LDA and GGA schemes, regardless of computational technique used, is about the same and in good agreement with the experimental value. The contribution from the core is negligibly small. This is because as these electrons are more tightly bound in diamond than in other semiconductors.

The positron affinity with the positron correlation potential treated in the LDA scheme (see Table II) is found to be close to the previous calculation of -2.5 eV (Ref. 35). The positron affinity at 0 K is estimated to be -0.8 eV from the measured electron and positron work functions of Brandes and Mills.[2] Since the present calculation is referred to the top of the valence band, it is required to take account of the electron Fermi energy due to the boron level (0.35 eV above the top of the valence band) in the experiment mentioned to compare it meaningfully with theory. The experimental value of A_+ referred to the top of the valence band is then -1.15 eV, which is smaller (in magnitude) than our result. Although the positron correlation energy based on the GGA scheme brings the theory closer to experiment (see Table IV), yet the difference is still about 1 eV, which is not negligible. When considering LMTO-ASA results (Table V), the difference is even larger. The reason for such a discrepancy is probably that the electron energy levels have not been evaluated in the presence of the boron impurity. The exact method would need a Car-Parrinello calculation for the determination of the electron energy levels where the lattice relaxation in the presence of the boron impurity is considered
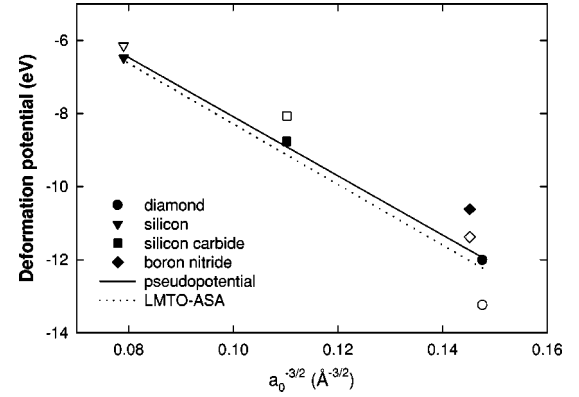

FIG. 1. The dependence of the positron deformation potential on the inverse of the square root of the cell volume in semiconductors studied. Filled symbols mark pseudopotential results. The same open symbols denote the respective LMTO-ASA results. See the text for an explanation of straight lines.

(cf. Ref. 30). The interpretation of the experiment is further complicated by the presence of hydrogen and oxygen at the diamond surface (see Ref. 2 for details).

The calculated deformation potential in the LDA scheme (Table II) is found to be slightly smaller than that given by an earlier pseudopotential calculation[36] which predicted it to be -12.3 eV. However, in that calculation the crystal zero scheme was based on the vanishing of the Coulomb potential at the Wigner-Seitz radius. The measured positron mobility, which is related to D_+ [see Eq. (1)], in the temperature range 300 K to 400 K shows that the positron scatters from the acoustic phonons.[37] In order to reproduce the experimental results, together with the deformation potentials calculated in the LDA and GGA schemes, the positron effective masses are $1.9m_e$ and $2.0m_e$, respectively. These effective masses do not seem to be reasonable. However, taking the above masses and deformation potential, it is possible to explain the experimental data[36] in the framework of the shallow trapping model.

B. Silicon

The positron lifetime in Si calculated using the pseudopotential method is in nearly perfect agreement with the experimental value of 216 ps (Ref. 27). With the positron correlation energy in the GGA scheme (Table IV) the lifetime is calculated to be slightly smaller than in the LDA formalism (Table II). Present LMTO-ASA calculations (cf. Ref. 27) give values smaller than those originating from the pseudopotential method, but the agreement with the experiment is still good.

The positron affinity in Si as given by the LMTO-ASA method within the LDA formalism is -7.17 eV (Table III; see also Ref. 35). In the present pseudopotential calculation the positron affinity obtained with the LDA positron scheme (Table II) is found to be shifted up with respect to the LMTO-ASA method. The experimental electron work functions in the [100] and [111] directions in Si were found[12] to be 4.91 eV and 4.74 eV, respectively. Taking the average electron work function as 4.82 eV and the positron work function -1 eV (Ref. 12), the positron affinity is estimated as -3.82 eV. The electron work function can also be esti-

mated from the electron affinity and band gap, which refers to the top of the valence band. This leads to an electron work function of 5.14 eV using the electron affinity 4 eV and band gap 1.14 eV. In this way we obtain the positron affinity as -4.14 eV. It is quite clear that neither experimental affinity is in agreement with the theory. This might be improved by taking into account the electronic polarization in calculations, as Pennetta[12] has argued. On the other hand, the experimental work functions can also be influenced by a defect site, as mentioned above.

The positron deformation potential in Si does not differ too much when calculated using the LMTO-ASA and pseudopotential techniques. The accurate experimental data by Mäkinen[38] have shown that the positron deformation potential is -6.2 ± 0.3 eV provided the positron effective mass is chosen to be $1.5m_e$. An earlier calculation[39] has determined the positron effective mass as $1.45m_e$. Thus the positron deformation potential calculated here is in good agreement with experiment.

C. Silicon carbide

Recently, the positron affinity has been measured[11] in $3C$, $4H$, and $6H$ polytypes of SiC and compared with theoretical results based on the LMTO-ASA method. The experimental results in these three different polytypes are quite similar. Therefore, here the positron lifetime, affinity, and deformation potential have been calculated in $3C$-SiC only and compared with experiment.

It should be mentioned that in Ref. 11 a different exchange-correlation potential[40] was employed in the electronic structure calculations. This fact turns out to be the origin of slightly distinct results for the positron affinity in the present work, namely, the present LMTO-ASA values of A_+ are shifted upward with respect to those presented in Ref. 11 by about 0.55 eV (see Tables III and V and Table II in Ref. 11). In any case, the LMTO-ASA values are still in strong disagreement with the experimental value of -3.83 ± 0.45 eV. Surprisingly, the present pseudopotential calculation of the positron affinity, when the GGA positron correlation energy is considered, agrees quite well with experiment.

The positron lifetime in $3C$-SiC calculated here agrees reasonably with the experimental value of 140 ps given for $6H$-SiC in Ref. 10 (we do not expect that the $3C$-SiC value will differ significantly from the $6H$-SiC one[10]). More specifically, the pseudopotential calculations slightly overestimate the experimental values, whereas the LMTO-ASA method gives slightly smaller values.

The experimental positron diffusion constant D_+ in SiC is found to vary in the range 0.3–0.8 cm^2 s^{-1} at room temperature.[41] The value of c_L [see Eq. (1)] in SiC is estimated as 4.79×10^{12} dynes cm^2. Taking the positron effective mass to be $1.5m_e$, the theoretical value of D_+ is found to vary in the range 3.6–3.8 cm^2 s^{-1} (taking into account values in Tables II and IV), which is much higher than the value given by experiment. LMTO-ASA calculations lead to even slightly higher values. This indicates that the acoustic phonon scattering is not important in SiC at room temperature. It has been found in GaAs that the positron scatters only with optical phonons in the temperature range 50–500 K (see

Ref. 42). From our results it appears that other scattering phenomena such as optical phonon scattering and ionized impurity scattering together with shallow trapping[36] are responsible for reducing the deformation potential in SiC.

D. Boron nitride

We have calculated the positron lifetime, affinity, and deformation potential in boron nitride. These positron properties for BN are close to those found for diamond. This is probably due to the similar lattice constants and atomic constituents in both semiconductors (the atomic numbers of B and N differ just by 1 from that of diamond), which results in a similar electron distribution as the background for determination of positron properties.

Recently, proposals[43–45] have appeared to use rare gas solids, diamond, and SiC as field assisted moderators. Various other semiconductors have also been examined with respect to this purpose in Ref. 46. The similarity of the calculated parameters of BN and diamond suggests that it is worth trying to study BN as a field assisted moderator as well.

IV. CONCLUSIONS

Positron lifetimes, affinities, and deformation potentials have been calculated in the LDA and GGA formalisms for diamond, Si, SiC, and BN and compared with available experimental data. Results are often found to be slightly different from those given by the conventional LMTO-ASA method. Positron lifetimes usually agree quite well with experimental data, which is not the case for positron affinities. Positron deformation potentials can usually be compared with experiment only indirectly using data about positron diffusion. Unfortunately, there are not yet enough experiments to compare and judge the accuracy of this work in detail. This is principally the case for boron nitride.

Regarding positron affinity calculations, we observe that the results depend only slightly on the treatment of electrons (LDA or GGA), but the GGA approach for positrons results in A_+ values that are apparently closer to experimental ones (if available) than those originating from the LDA approach. On the other hand, such an improvement is not sufficient, except for SiC and the pseudopotential method. This, in our opinion, indicates that even the GGA for positrons does not satisfactorily describe electron-positron correlations in semiconductors, as discussed in more detail in Ref. 11. We do not have any explanation for the relative success of the GGA in SiC, and further studies using precise electronic structure methods are needed to clarify this point. In this context, it is worth mentioning that even in metals, where the differences in A_+ values between theory and experiment are evidently smaller than in semiconductors, the situation is somewhat ambiguous,[27,28] as in $3d$ metals the GGA scheme for positrons improves the agreement of theory and experiment, but not in other d metals.

From the experimental point of view the determination of the positron affinity in semiconductors is a quite difficult task comprising measurement of electron and positron work functions. Various surface effects[2] can influence the resulting positron affinity, which is a critical issue for comparison with theory that determines the positron affinity as a bulk property not related to the surface. This point has to be dis-

cussed for every particular case as it depends on the system studied and also on the methods used to measure both work functions.

As concerns positron affinity measurements in general, there are not many semiconductors known having a negative positron work function, which is a prerequisite for such measurements. If the positron work function is positive, conventional positron emission spectroscopy method cannot be employed to determine the positron affinity. However, Weiss *et al.*[47] have proposed that the positron affinity for a sample with positive positron work function can also be measured from the kinetic edge of the positron induced secondary electron emission. Unfortunately, this method is not yet fully established to provide experimental affinity data in semiconductors.

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