

Predicted band offsets for 55 semiconductor heterojunctions

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Abstract

A rather general theory of heterojunction band offsets published recently by us is summarized and improved in some details. It is applied to 55 heterojunctions as possible combinations of 11 semiconductors. For 19 of them there exist reliable experimental values. Comparison with the experiment shows that the present theory yields a significantly better agreement with experiment than those of Tersoff and others. The present theory gives non-transitive band offsets in accordance with experimental observations. Thus for the 36 heterojunctions for which no experimental band offsets are available our predicted values can serve as a reasonable estimate. In addition also the completely independent values following from the electron affinity rule are given.

1. Introduction

The theory of heterojunction band offsets is the subject of numerous publications (for reviews see [1,2,3]). In these papers very different properties of the semiconductor, its surface or of the interface are assumed to be the dominating quantity determining the band offset. Probably the most frequently used expression for predicting band offsets was established by Anderson [4]. Although the accuracy of his electron affinity rule is only moderate it is wide-spread due to the availability of the data needed. A further development of the electron affinity rule is given in [5,6]. Other often cited theories [7,8,9,10] are based on the assumption of equalizing reference levels for the band edges of both semiconductors. These theories and the electron affinity rule yield a linear dependence of the band offset on bulk or surface properties. But linearity imposes a principal accuracy limit on the predictions. Other theories [5,11] are better justified from a theoretical point of view. Connections between these partly controversial descriptions were shown in detail recently [12].

In a previous paper [12] we presented a rather general theory on heterojunction band offsets. It is based on (i) using an exactly defined equilibrium condition, (ii) considering both the band bending and the microscopic charge redistribution at the interface which are both needed to reach equilibrium and (iii) taking into account the dependence of the charging of the gap states on the band bending. Already a first simplified estimate [12] led to an important improvement of the accuracy of the calculated band offsets compared to the predictions of Tersoff's theory [7] giving most accurate band offsets before.

The aim of this paper, besides improving the theory in some details, is mainly to predict band offsets for such cases where experimental results are not available. For the 55 heterojunctions

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considered surprisingly indeed only for 19 reliable measured values were published [1]. Comparison for these cases show the improvement reached with our description: the mean square and the maximum deviations from the experiment are 0.15 eV and 0.27 eV, respectively, whereas the corresponding values for Tersoff's theory are 0.21 eV and -0.37 eV and for the electron affinity rule 0.56 eV and 0.99 eV. These numbers have to be compared to the accuracy of the experimental values which was estimated to be ± 0.1 eV [1] (but this might be too optimistic, e. g. for Ge-GaAs photoemission measurements gave values for the valence band offset between 0.24 eV and 0.7 eV). Thus for these 36 heterojunctions where no experimental offsets are available our predicted values can serve as a quite reasonable estimate. Additionally we gave also the completely independent values following from the electron affinity rule since, of course, only the mean and maximum deviations are expected to be smallest for our values.

2. Theory

The valence band offset is by definition the difference of the valence band edges E_{vi} measured near the interface on the same (arbitrary) energy scale

$$\Delta E_v = E_{v2} - E_{v1}. \quad (1)$$

Lower indices $i = 1, 2$ are used for the semiconductor on the left and right half spaces, respectively. With the notation $\Delta E \equiv E_2 - E_1$ the conduction band offset is $\Delta E_c = \Delta E_v + \Delta E_g$ where E_g is the gap energy. Fig. 1 shows the schematic band diagram of the junction with the macroscopic band bendings V_{oi} (Debye-length scale) on both sides of the mathematical interface. The (electro-) chemical potential μ is constant throughout the contact and can be used as the common energy zero for determining the band offset. Then the valence band edges depend as $E_{vi} = \zeta_i - E_{gi} + V_{oi}$ on the band bending V_{oi} and the energetic distance ζ_i of the bulk conduction band edge ϵ_{ci} from the chemical potential

$$\zeta \equiv \epsilon_c - \mu = \epsilon_v + E_g - \mu. \quad (2)$$

Then the valence band offset is simply

$$\Delta E_v = \Delta \zeta - \Delta E_g + \Delta V_o. \quad (3)$$

In (3) the band bending V_{oi} is positive always if the bands are bent upwards in direction to the mathematical interface. According to (3) the so called "built-in potential" ΔV_o determines the band offset. But ΔV_o itself depends on the electronic structure of the immediate interface region which has therefore to be considered in detail.

Contacting two half-infinite solids results in a charge transfer in order to equalize the chemical potentials. The total interface dipole barrier P_o which is built up by this charge transfer is equal to the difference in the chemical potentials. But the (electro-) chemical potentials μ_i depend on the energy zero. If the required unique reference levels are denoted by $\varphi_{co,i}$, the interface dipole is given by

$$P_o = - (\mu_2^b - \mu_1^b) \quad \text{with} \quad \mu_i^b = \mu_i - \varphi_{co,i}. \quad (4)$$

It has been shown in [12] that the reference levels $\varphi_{co,i}$ are uniquely determined by the corresponding bulk charge density alone for a given surface orientation (and a given top atomic layer for a more complicated crystal structure). In semiconductors the chemical potential depends on doping and temperature. Therefore, the valence bulk band edge relative to the reference level

$$\epsilon_{vi}^b = \epsilon_{vi} - \varphi_{co,i} \quad (5)$$

is introduced. With (2) and (5) one can rewrite (4) as

$$P_o = -\Delta\varepsilon_v^b - \Delta E_g + \Delta\zeta. \quad (6)$$

Here doping and temperature influence mainly $\Delta\zeta$ alone. It should be emphasized that the value of the interface dipole barrier P_o (6) which has to be built up in order to achieve equilibrium is uniquely determined by the total bulk charge densities for a given interface orientation [12]. To evaluate P_o (6) one has to consider (2), (5), and the equations determining the reference levels $\varphi_{co,i}$ given elsewhere [12]. The charge transfer needed to obtain the dipole barrier P_o of the magnitude (6) consists of two contributions. At first one has a charge redistribution at the interface on an atomic length scale resulting in a contribution D_o . Secondly, there occur two space-charge layers and a net interface charge. The resulting band bending difference $V_{o1} - V_{o2} = -\Delta V_o$ also contributes to P_o . Therefore one has

$$P_o = D_o - \Delta V_o. \quad (7)$$

Evidently, only the part ΔV_o of (7) contributes to the band offset (3). On the other hand one can eliminate ΔV_o from (3) by using (7) and obtains for the band offset with (6)

$$\Delta E_v = \Delta\varepsilon_v^b + D_o. \quad (8)$$

Apparently, from (8) one could conclude that the only (self-consistent) interface property determining the band offset is the microscopic dipole barrier D_o at the interface. Indeed, this is the assumption underlying a large group of theories on heterojunction band offsets (see [6,12]). Actually, the macroscopic contribution ($-\Delta V_o$) and the microscopic one (D_o) to the dipole barrier P_o (7) are coupled with one another as will be explained in the following.

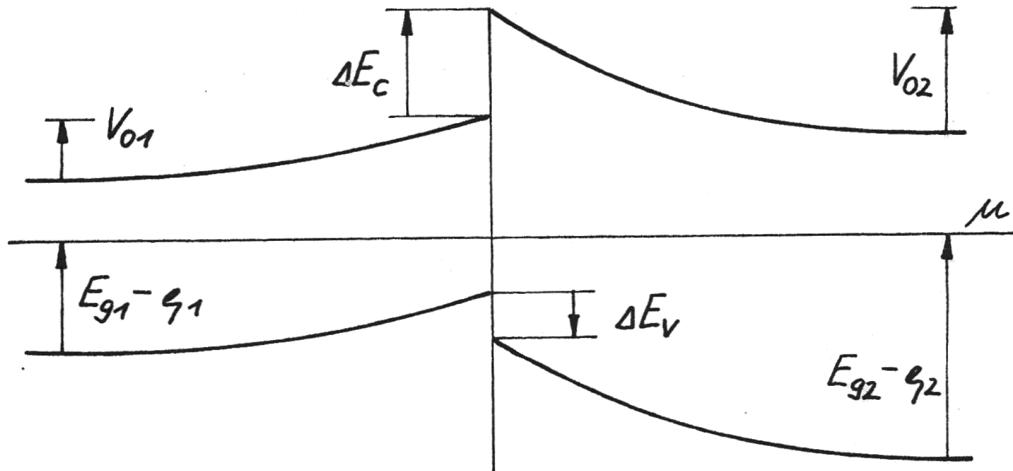


FIG. 1: Energy diagram of a heterojunction in the scale of the Debye screening length.

The microscopic interface contribution D_o to the interface dipole barrier can be regarded as consisting of two parts [13]:

$$D_o = D_e + D_{vs}. \quad (9)$$

D_e arises from the smooth matching of the valence bulk charge densities and D_{vs} is created by charged gap states at the interface. In order to evaluate the latter the concept of the neutrality level is used. The interface neutrality levels ϕ_{ni} (relative to the valence band edge at the interface) in the semiconductor i is defined such that the number of valence band states per unit area missing due to the boundary condition (compared to periodic boundary conditions) is compensated by

the decaying gap states in the gap below ϕ_{ni} . If the chemical potential coincides with ϕ_{ni} (i. e. $\phi_{ni} = E_{gi} - \zeta_i - V_{oi}$) one has local neutrality. All the corresponding states contribute to D_e . But usually the chemical potential deviates from ϕ_{ni} and one has a net charge per unit area [14] of decaying gap states

$$\sigma_{vsi} = -e N_{vsi} (E_{gi} - \zeta_i - V_{oi} - \phi_{ni}) \quad (10)$$

where N_{vsi} is the density of gap states near ϕ_{ni} [15]. The total charge

$$\sigma_{vs} = \sigma_{vs1} + \sigma_{vs2} \quad (11)$$

gives rise to the two space-charge layers connected with the band bendings. But there remains a microscopic dipole layer due to the charged gap states having the effective extensions δ_i . As shown in the appendix the latter produces a dipole barrier (eqs. (A5) with (A7))

$$D_{vs} = -\frac{e}{\epsilon_0} [\delta_2 \sigma_{vs2} - \delta_1 \sigma_{vs1}] . \quad (12)$$

Via σ_{vsi} (10) D_{vs} depends on the band bendings V_{oi} and hence on the band offset itself (see (3)). This dependence becomes more clear by combining (12) with (11) and considering (10) and (3). Then one obtains for (9)

$$D_o = D_e - \alpha (\Delta E_v + \Delta \phi_n) + \tilde{D}_{vs} \quad (13)$$

$$\alpha \equiv \frac{e^2 (\delta_1 + \delta_2)}{\epsilon_0} / \left[\frac{1}{N_{vs1}} + \frac{1}{N_{vs2}} \right] \quad (14)$$

$$\tilde{D}_{vs} = -\frac{e}{\epsilon_0} \left[\frac{\delta_2 N_{vs2} - \delta_1 N_{vs1}}{N_{vs2} + N_{vs1}} \right] \sigma_{vs} . \quad (15)$$

An expression similar to (13) was published earlier [5] but without \tilde{D}_{vs} (15) and without an explicit expression for α (14). Both were derived first by us.

Equations (13) and (8) show the coupling of the microscopic dipole barrier with the band offset (and due to (3) also with the band bendings). Both equations represent a negative feedback mechanism stabilizing the band offset. Solving the two equations for the band offset yields

$$\Delta E_v = \frac{1}{1+\alpha} \left[\Delta \epsilon_v^b + D_e + \tilde{D}_{vs} \right] - \frac{\alpha}{1+\alpha} \Delta \phi_n \quad (16)$$

together with the explicit expressions (14) and (15). It should be mentioned that apart from the small 0.01 eV uncertainty explained in the appendix the only approximation in (16) is the linearization used in (10). It is justified if each deviation $E_{gi} - \zeta_i - V_{oi} - \phi_{ni}$ of the chemical potential from the neutrality level is small compared to the gap width. Our estimates showed that indeed usually this quantity is less than $E_g/10$.

For using (16) to evaluate the band offset further approximations are needed. At first in most cases \tilde{D}_{vs} represents a negligible contribution to D_{vs} : Usually the quantities σ_{vsi} (10) have opposite signs and are comparable in magnitude $|\sigma_{vs}| \ll |\sigma_{vs1}|, |\sigma_{vs2}|$. In (15) the total charge σ_{vs} is multiplied by the term in brackets being comparable with δ_i if the gaps are not too much different. Then it is seen from (12) and (16) that usually $\tilde{D}_{vs} \simeq 0$ is a good approximation. Indeed, estimates have shown that \tilde{D}_{vs} is of negligible influence on the band offset. A little more serious is the lack of knowledge on the dipole barrier D_e due to the smooth matching of the valence band states (up to the lower neutrality level). But at the free surfaces where the density decreases to zero the corresponding barrier has a value of one or a few eV. Therefore D_e should

be much smaller and considering the factor $(1 + \alpha)^{-1}$ in (16) it will be neglected here as a rough estimate. For the neutrality levels ϕ_{ni} in (16) we use the effective mid-gap levels E_B of Tersoff [7]. For the valence band energies ε_{vi}^b the values ε_v^{FK} of Frensel & Krömer [8] can be used [12] as a rough estimate although they were obtained within another context. Thus, the approximations we use to evaluate (16) are

$$D_e + \tilde{D}_{vs} \simeq 0, \quad \varepsilon_v^b = \varepsilon_v^{FK} [8], \quad \phi_n = E_B [1]. \quad (17)$$

Finally one needs the value of α (14). A systematic two-band model for the imaginary band structure yields for the decay length (A7) in (14)

$$\delta = \frac{1}{2q \varepsilon_{vsr}} \simeq \frac{2\pi \hbar^2}{m_o E_g a} = \frac{9.57 \text{ eV} \text{ \AA}^2}{E_g a} \quad (18)$$

where $\varepsilon_{vsr} \simeq 2.5$ is chosen. m_o is the electron mass and a is the perpendicular lattice constant. The density of states in (14) is given by

$$N_{vs} \simeq \frac{2}{\pi a^2 E_g}. \quad (19)$$

All data needed are summarized in Tab. 1. For these 11 semiconductors both the values ε_v^{FK} and E_B are available. InAs is not included since the effective mid-gap level E_B lies always in the conduction band ($E_B > E_g$).

TABLE 1: Values for calculating the band offsets (N_{vs} in $10^{18} \text{ m}^{-2} \text{ eV}^{-1}$)

sem.	E_g (eV)	a (\text{\AA})	δ (\text{\AA})	N_{vs}	ε_v^{FK} (eV)	E_B (eV)	ϕ_{PE} (eV)
Ge	0.67	5.658	2.524	2.968	-3.25	0.18	4.80
GaSb	0.72	6.094	2.181	2.381	-3.89	0.07	4.85
Si	1.11	5.431	1.587	1.944	-3.16	0.36	5.12
InP	1.26	5.869	1.294	1.467	-4.58	0.76	5.70
GaAs	1.43	5.642	1.186	1.399	-3.96	0.50	5.50
CdTe	1.44	6.477	1.026	1.054	-4.90	0.85	5.78
AlSb	1.60	6.136	0.975	1.057	-3.94	0.45	5.27
AlAs	2.15	5.661	0.786	0.924	-3.96	1.05	6.00
ZnTe	2.26	6.101	0.694	0.757	-4.74	0.84	5.78
GaP	2.27	5.450	0.773	0.944	-4.12	0.81	6.05
ZnSe	2.67	5.667	0.632	0.742	-5.07	1.70	6.80

3. Band offsets and electron affinity

The electron affinity χ_s is a property of the free semiconductor surface. It is measured via the photoemission threshold $\phi_{PE} = \chi_s + E_g$ [16]. For energetically characterizing the free surface in addition the work function ϕ_s is needed. Both are connected with one another and with the band bending V_s by

$$\phi_s = \chi_s + V_s + \zeta. \quad (20)$$

On the other hand the work function consists of [17] a dipole barrier ($V_s + D_s$) (similar to (7) D_s is caused by a charge redistribution on an atomic length scale), and the bulk chemical potential (4) according to

$$\phi_s = (V_s + D_s) - \mu^b = (V_s + D_s) - (\zeta - \varepsilon_v^b - E_g) \quad (21)$$

where in the second equation (2) and (5) are used. From (20) and (21) we obtain for the affinity

$$\chi_s = D_s - \varepsilon_v^b - E_g. \quad (22)$$

Finally, inserting (22) into (8) one obtains as an exact expression for the band offset

$$\Delta E_v = -\Delta \chi_s - \Delta E_g + (D_o + D_{s2} - D_{s1}) \quad (23)$$

containing the electron affinity rule. The microscopic interface and surface dipole barriers D_o and D_{si} , respectively, are not available from experiment. To obtain Anderson's affinity rule [4]

$$\Delta E_v = -\Delta \chi_s - \Delta E_g = -\Delta \phi_{PE}. \quad (24)$$

one has to assume $D_o = D_{s1} - D_{s2} = -\Delta D_s$. This means just superposition of the two surface barriers D_{si} to built up the interface barrier. Deviations from this simple superposition are the reason for the only moderate agreement of (24) with the experimental values (see Tab. 2). The derivation given here shows the actual approximation needed to obtain Anderson's rule (24). His original arguments can be discussed better combining (20) with (3) giving

$$\Delta E_v = -\Delta \chi_s - \Delta E_g + (\Delta \phi_s + \Delta V_o - \Delta V_s). \quad (25)$$

Eq. (24) is valid if only a change of the band bendings occurs when the two semiconductors with free surfaces are brought together. Then, of course, one has also the superposition of the microscopic dipole barriers. (Comparison of (25) with (23) shows that the last term in both equations must be the same.) So the flat band case ($V_{si} = 0$) is not required for the validity of (24) as stated earlier [12].

4. Numerical results

As already mentioned reliable values for ε_v^{FK} and E_B needed to evaluate the band offset with the theory outlined in Section 2 using (16) with (17) – (19) are available for 11 semiconductors (Tab. 1). Consequently the band offsets were calculated for 55 heterojunctions corresponding to the possible combinations of these 11 semiconductors. But in addition the electron affinity rule (24) gives the possibility for a further independent estimate. According to the compilation [1] reliable experimental values are available for 19 of these 55 heterojunctions. In Tab. 2 for each pair of semiconductors 2–1 the valence band offsets $\Delta E_v = E_{v2} - E_{v1}$ are given. The first row contains the available experimental values, in 6 cases the smallest and the largest are given, since different values are published. In the second row our values according to (16) and in the third row those following from the electron affinity rule (24) are given.

Already a first simplified evaluation [12] of (16) yielded the best agreement with the experimental values, also better than the Tersoff [7] theory. Here we improve our predictions furthermore. The mean square and maximum deviations from the 19 experimental values (mean values if different values are published) are only 0.15 eV and 0.27 eV, in the case of the electron affinity rule 0.56 eV and 0.99 eV, respectively (Tersoff [1]: 0.21 eV and -0.37 eV). The accuracy of the experimental values itself is not better than 0.1 eV. Therefore in the larger number of cases where no experimental values are known our results can be regarded as reasonable predictions for the band offsets. In addition one can consider the values of the electron affinity rule (the mean and maximum deviations from experiment are larger, nevertheless in special cases this estimate can be better).

TABLE 2: Band offsets $\Delta E_v = E_{v_2} - E_{v_1}$ for 55 heterojunctions: upper value: experiment [1], middle value: this theory, lower value: electron affinity rule [4,6] (all values in eV)

	ZnSe (1)	GaP (1)	ZnTe (1)	AlAs (1)	AlSb (1)	CdTe (1)	
Ge (2)	1.29–1.52	0.80	0.95	0.78–0.95	–	0.85	exp this EA
	1.59	0.68	0.84	0.84	0.34	0.83	
	2.00	1.25	0.98	1.20	0.47	0.98	
GaSb (2)	–	–	–	–	0.4	–	
	1.51	0.63	0.79	0.78	0.32	0.82	
Si (2)	1.95	1.20	0.93	1.15	0.42	0.93	
	–	–	–	–	–	0.75	
	1.25	0.80	0.85	–	–	0.75	
	1.52	0.59	0.82	0.72	0.26	0.79	
	1.68	0.93	0.66	0.88	0.15	0.66	
InP (2)	–	–	–	–	–	–	
	0.77	–0.11	0.11	0.00	–0.40	0.15	
	1.10	0.35	0.08	0.30	–0.43	0.08	
GaAs (2)	0.96–1.1	–	–	0.15–0.45	–	–	
	1.17	0.26	0.50	0.37	–0.04	0.52	
	1.30	0.55	0.28	0.50	–0.23	0.28	
CdTe (2)	–	–	–	–	–	–	
	0.56	–0.32	–0.07	–0.24	–0.59	/	
	1.02	0.27	0.00	0.22	–0.51		
AlSb (2)	–	–	–	–	–	0.20	
	1.20	0.29	0.57	0.37	/	–0.05	
	1.53	0.78	0.51	0.73		0.05	
AlAs (2)	–	–	–	–	–0.05	0.17–0.4	
	0.87	–0.07	0.26	/	0.17	0.15	
	0.80	0.05	–0.22		0.27	0.32	
ZnTe (2)	–	–	–	0.57	–	0.64	
	0.58	–0.31	/	0.59	0.69	0.68	
	1.02	0.27		0.58	0.85	0.90	
GaP (2)	–	–	–	0.05	–	0.23–0.7	
	0.92	/	–0.35	0.27	0.37	0.37	
	0.75		–0.20	0.38	0.65	0.70	
	GaAs (2)	InP (2)	Si (2)	GaSb (2)	Ge (2)		

Finally some remarks on different influences on the band offset will be made. (i) It is very important that contrary to previous theories but in agreement with the experiment [2] our values for the band offset are not transitive ($\Delta E_v^{3,1} \neq \Delta E_v^{3,2} - \Delta E_v^{1,2}$). In our theory the non-transitivity is a result of the non-transitivity of α (14). (ii) In agreement with the experiment the band offset is independent of the doping levels, or the values of ζ : A change of $\Delta\zeta$ is compensated by an opposite change of the band bendings ΔV_o (see also the remark in the appendix on the boundary condition for solving Poisson's equation in the space-charge layers). Deviations are possible only if dopants segregate at the interface. (iii) Experimentally there is no definite information on the orientation

dependence of the band offset. Principally via $\Delta\varepsilon_v^b$ in (16) our theory contains such a dependence since the reference level in (5) depends so. For the band offset this dependence is reduced by the factor $(1 + \alpha)^{-1}$. A quantitative estimate would require to determine the orientation dependence of the reference level with the method described by us [12]. (iv) Improvements concern mainly better estimates for D_e and possibly for ε_v^b in (16).

Appendix: Dipole barrier due to charged gap states

In both semiconductors i one has charged gap states with a net charge per unit area (10) contributing to the total charge (11). In fact the charged gap states have a spatial extension perpendicular to the interface being described by a charge density $\varrho_{vs,i}(z)$. So one has

$$\sigma_{vs,i} = \int dz \varrho_{vs,i}(z). \quad (A1)$$

$\varrho_{vs1}(z)$ is zero in the semiconductor 2 and vice versa. The total charge is simply

$$\sigma_{vs} = \int dz \varrho_{vs} \quad \text{with} \quad (A2)$$

$$\varrho_{vs}(z) = \varrho_{vs1}(z) + \varrho_{vs2}(z). \quad (A3)$$

Now it is convenient to rewrite (A3) as

$$\varrho_{vs}(z) = [\varrho_{vs}(z) - \sigma_{vs} \delta(z)] + \sigma_{vs} \delta(z). \quad (A4)$$

($\delta(z)$ is the Delta-function.) Here the first term in brackets is a neutral dipole layer due to (A2) whereas the second term is an interface charge per unit area being equal to the net charge (11). This second term will be screened by space-charge layers on both sides of the interface. The resulting band bendings V_{o1}, V_{o2} follow from solving Poisson's equation. As usual the first boundary condition is that σ_{vs} determines the discontinuity of the electric field across the junction. But a peculiarity is the second boundary condition: instead of continuity of the potential one has to consider the discontinuity of the band edges, that means the band offset. The first term on the right hand side of (A4) gives rise to a dipole barrier which is clearly found to be

$$D_{vs} = -\frac{e}{\varepsilon_o} (\tilde{\delta}_2 \sigma_{vs2} - \tilde{\delta}_1 \sigma_{vs1}) \quad (A5)$$

with the decay lengths

$$\tilde{\delta}_i = \left| \int dz z \varrho_{vs,i}(z) \right| / \int dz \varrho_{vs,i}(z) \quad (A6)$$

of the charged gap states. It can be approximated by the exponential decay length $(2q)^{-1}$ of the gap states near the neutrality level. But in addition a screening of these states should be taken into account [18]. Then one has

$$\tilde{\delta} \rightarrow \delta = \frac{1}{2q \varepsilon(2q)} \quad (A7)$$

where $\varepsilon(2q)$ is the dielectric function appropriate to this decay length. A reasonable estimate seems to be $\varepsilon(2q) \simeq 2.5$ for most semiconductors (see [18]).

The procedure presented here shows clearly a principal uncertainty in splitting up the dipole barrier (7) into band bending difference and a microscopic contribution. The band bendings result from the last term of (A4). But in (A4) the plane $z = 0$ for the net interface charge is to some extent arbitrary. It could be shifted within the two decay lengths. This would result in a change of (A5) and an opposite one in the difference of the band bendings. This uncertainty is therefore just the change of the band bending over the decay length of the gap states. It can be estimated

to be smaller than 10 meV.

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