I. INTRODUCTION

The identification and design of high-efficiency all-semiconductor spin-filtering devices, which operate at room temperature and zero external magnetic field, are of profound interest for spintronic applications. In spite of some success, for example, regarding improved spin injection from ferromagnets into Si, progress has been moderate. Diluted magnetic semiconductors, such as GaMnAs, which have been grown most successfully with good interfacial quality onto nonmagnetic zinc-blende (ZB) semiconductors, have been studied by Bengone et al. These authors concluded that $A_{Ga}$ and $A_{Cr}$ antisite defects have a minor influence on the transmission function. Interfacial defects and disorder at the GaAs-CrAs interface have been investigated theoretically elsewhere. Furthermore, experimental work on the magnetic and electrical properties of ZB CrAs, the growth parameter dependence of the magnetic properties of thin film CrAs, and the initial adsorption of Cr atoms on GaAs(0,0,1) has been reported. Wang et al. even report the growth and characterization of ZB CrAs/GaAs/MnAs/GaAs multilayers. Yamada et al. have investigated the magnetic properties of thin film (Ga, Cr)As.

Recently, the effect of electronic correlations upon the half-metallicity of stacked short period (CrAs)$_{\ell}$/GaAs$_{\ell}$ ($\ell \leq 3$) superlattices along [001] has been investigated. Results indicate that the minority spin half-metallic gap is suppressed by local correlations at finite temperatures and continuously shrinks on increasing the heterostructure period. As a consequence, at the Fermi level, the polarization drops continuously shrinks on increasing the heterostructure period. As a consequence, at the Fermi level, the polarization shrinks on increasing the heterostructure period. As a consequence, at the Fermi level, the polarization shrinks on increasing the heterostructure period. As a consequence, at the Fermi level, the polarization shrinks on increasing the heterostructure period. As a consequence, at the Fermi level, the polarization shrinks on increasing the heterostructure period. As a consequence, at the Fermi level, the polarization shrinks on increasing the heterostructure period.
different layers, which may be detected in photo-absorption measurements.

Another density-functional theory (DFT) based calculation, as well as an experimental report have lead to the claim that the ZB-structure of thin film CrAs is energetically unstable.\textsuperscript{11,31} It was argued that the experimentally observed ferromagnetic behavior reported in Refs. 14, 15, and 17 may be caused by magnetic defects near the heterointerface and that no half-metallicity may be present at all. An additional problem to our knowledge, not studied in detail as of yet, may be the uncontrollable diffusion of Cr into GaAs thereby forming deep traps.\textsuperscript{32} It has to be noted that the final answer to the structural properties and stability of thin films of CrAs on top of GaAs, as well as CrAs/GaAs heterostructures, can only be given by or in conjunction with further experiments. It is indeed the aim of this article to stimulate these experimental studies by demonstrating that epitaxial CrAs/GaAs heterostructures should function as very efficient all-semiconductor room-temperature spin-filtering devices.

Exploring spin-filtering in GaAs-CrAs-GaAs heterostructures, first we investigate the stability of the CrAs unit cell under longitudinal distortion. It is a central result of this work that a tetragonal, local-minimum bulk phase of CrAs can be found, which is very near to being ZB lattice matched to bulk GaAs. This implies that one may perform transport calculations under the assumption of perfect ZB lattice matching without introducing a large systematic error. The band alignment is determined within our LSDA approach with the help of two different approaches, which both yield rather similar results. This provides a reasonable error estimate for the method employed, and leads us to the conclusion that half-metallicity in CrAs is not a necessary ingredient for efficient spin-filtering. In this conclusion, we may differ from that previous analysis of CrAs/GaAs trilayers.\textsuperscript{22} Rather, the interfacial properties and the spin-selective band alignment between the CrAs and GaAs layers appear to be essential. We map the electronic structure of the bulk materials onto an effective 20-orbital sp\textsuperscript{3}d\textsuperscript{5}s* nearest-neighbor empirical tight-binding (ETB) model, which is, particularly, suited for non-equilibrium transport calculations.\textsuperscript{33–36} In a final step, we calculate the spin-selective non-linear current-voltage (I–V) characteristics within the non-equilibrium Green’s function formalism for different layer thicknesses and temperatures. In summary, improvements and novelties over previous work involve: a combined determination of the spin-sensitive electronic structure within LMTO-ASA, determination of the band-alignment, identification of a local-minimum (tetragonal) CrAs structure with \( d_0 = d_{\text{GaAs}} \), a tight-binding matching without additional (ad-hoc) parameters making use of the common anion As, and transport calculations beyond linear response.

This article is structured as follows. In Sec. II, we summarize the theoretical approach and present the results for the electronic structure within the linear muffin-tin orbital (LMTO) method. In Sec. III, we describe the mapping procedure onto the tight-binding model. The transport model and results for the spin-current response are discussed in Sec. IV. Summary and conclusions are given in Sec. V.

II. LMTO ELECTRONIC STRUCTURE CALCULATIONS AND THE ZB CrAs/ZB GaAs [1,0,0] BAND-ALIGNMENT

The electronic structures of bulk ZB GaAs, bulk ZB and tetragonal CrAs, as well as that of several CrAs/GaAs supercells, have been determined employing the LMTO-ASA code, as developed by Jepsen and Andersen.\textsuperscript{37,38} A closely related code has been used previously to explore the electronic structure of bulk ZB CrAs and thin-layer ZB GaAs/CrAs superlattices. In particular, the half-metallic behavior as a function of superlattice period and lattice constants has been investigated.\textsuperscript{29,39} Details of this approach, as well as its benefits and caveats, can be found in the literature.\textsuperscript{38}

Our supercells, e.g., for (CrAs)\textsubscript{6}/(GaAs)\textsubscript{6}, extend along the [001] direction of the of bulk ZB material. The unit cells of the superlattice having the space group symmetry \( D_{2d}^1 \) are simple tetragonal with, for this case, \( c_0/a_0 = 12/\sqrt{2} \), where \( c_0 \) is the unit-cell dimension along the stacking direction. The bases of the tetragonal cell have the constants \( a = b = a_0/\sqrt{2} \), where \( a_0 \) represents the fcc lattice parameter. In our calculations, we use the lattice parameter \( a_0 = a_{\text{GaAs}} = 5.65\text{Å}, \) i.e., the experimental GaAs lattice parameter, unless stated otherwise. For open structures, such as ZB GaAs, it is customary to include empty spheres. For the bulk calculations, we consider two empty spheres and we use them in the heterostructure calculations as well. Atomic sphere radii are taken as 2.54 a.u. for Cr/E1 (first empty) and 2.70 a.u. for As/E2 (second empty).\textsuperscript{38} Our results do not change significantly even if we consider the radii to be equal to the average Wigner Seitz value of 2.62 a.u.

The electronic structure model is based on the local spin-density approximation (LSDA) omitting spin-orbit interaction and corrections for strong correlations as provided, for example, by the dynamic-mean-field-theory\textsuperscript{40} or the variational cluster approach.\textsuperscript{41,42} However, it has been shown by Chioncel et al.\textsuperscript{29,39} that the inclusion of correlations does not affect the magnetization and only leads to minor corrections to the band structure. It is well known that LSDA or its gradient-corrected approximation produce band gaps that are typically at least 30\% smaller than the experimental values for almost all semiconductors and insulators. In our case, too, the experimentally verified GaAs band gap of 1.52 eV at low temperatures is strongly underestimated by the present DFT method, predicting a value of about 0.35 eV. However, the overall features in the vicinity of the band gap are reproduced reasonably well. Since we do not study transport across the main energy gap, such as in Zener tunneling, this shortcoming is without any further disadvantage. Therefore, in what follows we consider two distinct cases: (i) we leave the electronic structure unchanged, i.e., we use the GaAs band structure with the underestimated band gap, and (ii) we scissor the GaAs electronic structure to the experimentally observed value of 1.52 eV. As we shall see, this does not affect the statement that CrAs/GaAs heterostructures function as spin-filters. Furthermore, we consider n-doped GaAs such that the spin-orbit effects, at least in GaAs, can be neglected. In the case of half-metals, one may speculate that the problems of LSDA are not as serious, since the dielectric response of half-metals is of...
metallic type. Previous results have shown that the detailed nature of states around \(E_F\) in bulk CrAs is changed when different lattice constants or models for electronic correlations are considered, while the overall features of the electronic structure are preserved.\(^{30}\) Clearly, the final answer as to the accuracy of the electronic structure model can only be given by comparison to experiment.

Since the GaAs band structure is well known and, except for the band gap, is fairly well reproduced within the LMTO-ASA code, here we confine ourselves to results obtained for CrAs. In a first approach, we assume that the ZB CrAs lattice constant is equal to the GaAs lattice constant \(a_{\text{GaAs}} = 5.65\,\text{Å}\). This choice is motivated by the hope that thin layers of CrAs can be grown onto a GaAs substrate in lattice-matched fashion. The electronic structure for majority and minority carriers is shown, respectively, in Figs. 1 and 2 (red solid lines). For the minority carriers, a gap of about 1.8 eV is predicted. A more detailed analysis of the electronic structure shows the origin of the valence band edge in the As-p–Cr-d hybrid orbitals, while conduction band edge states are dominated by the Cr-d orbitals, see Chioncel et al.\(^{29,39}\) Further, we observe from the ab-initio calculations that the lattice constant chosen for bulk ZB CrAs determines whether CrAs is half-metallic or not, see also Refs. 29 and 39. Since the bulk band structures of GaAs and CrAs combined in a heterostructure are shifted relative to each other by the computed band-alignment, as discussed below, we are led to the conclusion that half-metallicity of the CrAs layer is not compulsory for the realization of a spin-filter. A necessary ingredient, however, is the highly spin-dependent CrAs band structure.

We now investigate the total energy of the bulk CrAs unit cell as a function of the longitudinal, i.e., the out-of-the-plane, lattice constant \(a_\perp\), while holding the in-plane lattice constant \(a_\parallel\) fixed to \(a_{\text{GaAs}} = 5.65\,\text{Å}\), thus, making the unit cell tetragonal. It is reasonable to assume that, for thin lattice-matched layers of CrAs on top of GaAs, the in-plane lattice constant \(a_\parallel = a_{\text{GaAs}}\) takes on the value of bulk GaAs, i.e., that the in-plane symmetry is preserved. It is found that the minimal energy is achieved for 98% of the GaAs lattice constant, as depicted in Fig. 3, i.e., \(a_\perp = 0.98a_\parallel\). Hence, the actual unit cell of CrAs on the GaAs [1,0,0] surface is not perfectly cubic but tetragonal. The mere existence of such a (local) minimum close to the GaAs lattice constant is non-trivial and an important result and motivation for the spin transport analysis to follow. Moreover, a comparison of the bands of ZB CrAs with the bands of tetragonal CrAs with \(a_\perp = 0.98a_\parallel\) reveals that the electronic structure is almost unaffected by this distortion, see Figs. 4 and 5. Therefore, the systematic error introduced by assuming that the CrAs unit cell is perfectly cubic with \(a_\perp = a_\parallel = a_{\text{GaAs}}\), is negligible when compared to other uncertainties. We shall from now on assume that bulk CrAs (on [1,0,0] GaAs) has the ZB crystal structure.

In the spirit of core level spectroscopy, the band alignment at the [1,0,0] GaAs/CrAs interface was determined using the energy of a low-lying reference state that is present in both bulk materials, as well as in the CrAs/GaAs supercell. We chose two different reference states and compared the values obtained with each of them in order to have a reasonable error estimate for the method. The band offset parameter \(\Delta\) for the reference state is calculated according to Ref. 43.
spin-dependent. In the calculations below we chose $\Delta_1 = 0.60 \, \text{eV}$ and $\Delta_2 = 0.55 \, \text{eV}$, respectively, for majority and minority spins, as obtained within the method based on the As-3 s reference states.

In Figs. 1 and 2, we show on top of the electronic structure of majority- and minority-spin CrAs, the electronic structure of GaAs for case (i) (un-scissored gap) and case (ii) (scissored gap) taking into account the band offset. It can now clearly be seen that carriers injected from n-GaAs near the $\Gamma$-point do not reach the main energy gap region of bulk CrAs. Even in case of p-doping of the GaAs contact layers, this region can only be reached under an applied bias exceeding approximately 0.3 V, as can be observed from an inspection of Fig. 2. Moreover, scissoring of the GaAs band gap does not significantly change the spectral overlap of the lowest GaAs conduction band with the CrAs bands near the $\Gamma$ point. The situation is rather different for minority carriers, however. Here, the overlap of the lowest GaAs conduction band occurs, in both cases, with fairly flat CrAs bands of low mobility. Hence, the actual value of the band offset is not too important, which allows the claim that the presence of half-metallicity in the CrAs layer is not mandatory for spin-filtering in CrAs/GaAs heterostructures. In view of these results and the broad-band form of the electronic structure of CrAs in the relevant energy window, in particular, it appears that spin-filtering is rather stable with respect to moderate modifications to the value of the band offsets arising, for example, from interfacial defects or local lattice distortions.

III. EFFECTIVE sp$^3$d$^5$s$^* \text{ TIGHT-BINDING MODEL}

The results obtained within the LMTO electronic structure investigation encourage one to go one step further and to investigate spin-selectivity in the electric current for CrAs/GaAs heterostructures under bias. Since the LMTO calculations are based on thermal equilibrium, we first map the relevant segments of the electronic structure onto an ETB model on which we then base the non-equilibrium transport study. Specifically, each of the ab-initio electronic structure $\epsilon_{n}^{\text{LSDA}}$ of GaAs and of majority- and minority-spin CrAs are mapped onto an effective sp$^3$d$^5$s$^*$ nearest-neighbor ETB model.\cite{44–46} We chose an ETB model because it is particularly well-suited for non-equilibrium steady state transport calculations with the help of Green’s functions.\cite{33–36}

In principle, this step can be avoided if the LSDA wave functions were used to express the transmission function of the heterostructure, as, for example, proposed within the SIESTA DFT approach.\cite{47} The trade-off of an approach, which is based on the L(S)DA one-particle wave functions, however, is that its validity ad-hoc is questionable, since the wave functions used in the Kohn-Sham variational principle do not allow a direct physical interpretation. Their connection to the S-matrix of the (many-body) system is not obvious. The use of ground state wave-functions definitely limits one to the linear-response regime, since the transmission function would be obtained for zero external bias only. In general, L(S)DA bulk band structure calculations do not produce the correct energy gap. A simple scissoring strategy cannot be performed for a heterostructure, thus, any
deficiencies in the ab-initio electronic structure are carried over inevitably into the transport calculation. These difficulties have convinced us to follow a mapping approach from the ab-initio band structure calculation to an empirical tight-binding model and to take care of the interface problem in an additional step.

A mapping of the electronic structure onto an ETB model does not, in the first place, introduce any further systematic error, as long as the electronic structure in the relevant energy region is well approximated. Moreover, this approach comes with further benefits, such as computational effectiveness. It does not only allow one to account for known deficiencies of the electronic structure within DFT, such as a scissoring of the GaAs main band gap to the experimentally verified value, but also to control the particular modeling of the interface (e.g., by the inclusion of defects) and to treat a genuine non-equilibrium situation self-consistently. Bias-dependent mean-field corrections or disorder effects can be added in self-consistent fashion, as utilized by some of us recently for similar systems.48,49

The formal mapping process for a given bulk material is executed using a genetic algorithm, as implemented in Matlab, to minimize the cost functional

\[ K(\tilde{\xi}) = \sum_{n k} a_n(k) \left[ E_{SDA}^n(k) - E_{ETB}^n(k, \tilde{\xi}) \right]^2. \] (2)

Here, \( a_n(k) \) are normalized weights, where \( n \) is the band index and \( k \) is the wave vector, \( \tilde{\xi} \) denotes the set of 31 independent ETB parameters in the \( sp^3d^5s^* \) basis,44 and \( E_{ETB}^n(k, \tilde{\xi}) \) is the ETB band structure as a function of \( k \) and \( \tilde{\xi} \). The weights \( a_n(k) \) are used to restrict and focus the fit to the part of the band structure which contributes to charge transport. This ensures that the energy bands are well represented by the ETB fit and no “spurious bands” appear inside a chosen energy window.

Subsequently, the Hamiltonian of a given heterostructure can be put together layer by layer in a straightforward fashion. This convenient layer-by-layer construction can be carried over to the construction of the non-equilibrium Green’s function components and has been used in the calculations below. A further advantage is that we know the \( k \)-dependence of the bulk ETB Hamiltonian matrices analytically via the structure factors.44 Hence, the influence of small deviations in the ETB binding parameters can be investigated systematically.

One problem, however, arises when the interface between GaAs and CrAs has to be modeled in this modular approach.50 Let us briefly discuss the problem of how to model the interface in an adequate way, consistent with the available information, which are the ETB bulk Hamiltonians and the band offsets. The standard approach is to invoke the virtual crystal approximation (VCA).33,34,36,52-55 It has been demonstrated that this approximation is, in general, inconsistent since it violates symmetries underlying the bulk ETB Hamiltonians.50 In particular, the ETB parameters are not uniquely defined by the electronic structure alone; however, the VCA requires a unique identification of the ETB parameters.50 There are two possible remedies to this apparent inconsistency. First, we can formulate matching conditions which are a discrete form of the matching conditions in continuous space quantum mechanics. This approach works for pairs of band-to-band transitions and has been discussed extensively by Stickler and Pötz.50 Here, in this more complex situation, we shall follow an alternative approach made possible by the presence of As as a common anion: we can ensure that the ETB parameters can be uniquely attributed to one atomic species by posing a further constraint onto the fitting procedure Eq. (2): We require the As onsite energies (under zero bias and band offset) to be constant throughout the device. This is in accordance with ETB theory.44 Hence, the mapping onto a ETB model is executed in two steps: In a first step, we fit the majority and minority spin band structure of CrAs independently without any further restrictions. In a second step, we fit the GaAs band structure under the constraint that all As onsite energies have to have the same value as in CrAs. Let us briefly discuss the implications of such a fitting procedure: First of all, we obtain two different sets of ETB parameters for GaAs since we fit the two CrAs band structures independently and then restrict the GaAs parameters depending on spin orientation. Had we included the spin-orbit interaction into our model, two distinct sets of ETB parameters for GaAs would come more natural, however, in any case, the values obtained must be considered best fits under given constraints. Moreover, we emphasize that the particular form of the ETB parameters has no influence on the transport as long as the electronic structure including the band offset is reproduced reasonably well.50

All in all, we perform the down-folding process for four different combinations: (A) majority-spin CrAs and scissored GaAs, (B) majority-spin CrAs and un-scissored GaAs, (C) minority-spin CrAs and scissored GaAs, and (D) minority-spin CrAs and un-scissored GaAs. The ETB parameters which were identified as optimal for each of the four cases are listed in the Table I of the Appendix. The fits for GaAs together with the ab-initio band structure and the fits of majority- and minority-spin CrAs are given in Figs. 6–9. In view of the fact that the computed ab-initio electronic structure will have an inevitable inconsistency. First, we can formulate matching conditions which are a discrete form of the matching conditions in continuous space quantum mechanics. This approach works for pairs of band-to-band transitions and has been discussed extensively by Stickler and Pötz. Here, in this more complex situation, we shall follow an alternative approach made possible by the presence of As as a common anion: we can ensure that the ETB parameters can be uniquely attributed to one atomic species by posing a further constraint onto the fitting procedure Eq. (2): We require the As onsite energies (under zero bias and band offset) to be constant throughout the device. This is in accordance with ETB theory. Hence, the mapping onto a ETB model is executed in two steps: In a first step, we fit the majority and minority spin band structure of CrAs independently without any further restrictions. In a second step, we fit the GaAs band structure under the constraint that all As onsite energies have to have the same value as in CrAs. Let us briefly discuss the implications of such a fitting procedure: First of all, we obtain two different sets of ETB parameters for GaAs since we fit the two CrAs band structures independently and then restrict the GaAs parameters depending on spin orientation. Had we included the spin-orbit interaction into our model, two distinct sets of ETB parameters for GaAs would come more natural, however, in any case, the values obtained must be considered best fits under given constraints. Moreover, we emphasize that the particular form of the ETB parameters has no influence on the transport as long as the electronic structure including the band offset is reproduced reasonably well.

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best capture the overall features of the actual electronic band structure, the ETB fits achieved are highly satisfactory.

In principle, the spin-orbit interaction can be included in the ETB model following the work of Chadi. However, since the LMTO-ASA code itself currently does not feature spin-orbit interactions, its implementation at the ETB level would require the introduction of further (and somewhat arbitrary) parameters into our model, in particular, for CrAs. Furthermore, we shall focus on transport with n-doped GaAs buffer layers so that a detailed account of the spin-orbit interaction in the GaAs electronic structure will not really be important here.

IV. STEADY-STATE TRANSPORT

The I–V-characteristics of the heterostructure are calculated within a non-equilibrium Green’s function approach, which have been adapted from our recent study of GaMnAs-based heterostructures, to which we refer for further details and references. The Hamiltonian of the GaAs-CrAs-GaAs heterostructure is obtained by performing a partial Wannier transformation from the wave vector $k$ to $(x, k_{||})$, where $x$ denotes the [1,0,0] growth direction of the crystal and $k_{||}$ is the in-plane (parallel) $k$-vector

$$|nbjk_i\rangle = \frac{1}{L_{BZ}} \int dk_x \exp \left(-ik_x \frac{d_x}{4} \right) |nbk\rangle,$$

where $L_{BZ} = \frac{2\pi}{T_{k_{||}}}$ with $j$ labeling the atomic layer. The resulting one-particle Hamiltonian is of the single-particle form

$$H(k_{||}) = \sum_{i,\sigma} \varepsilon_{\sigma}^{(i)}(k_{||}) c_{i,\sigma}(k_{||})^\dagger c_{i,\sigma}(k_{||}) + \sum_{i,\sigma} \varepsilon_{\sigma}^{(i)}(k_{||}) c_{i+1,\sigma}^\dagger(k_{||}) c_{i,\sigma}(k_{||}) + \text{h.c.}$$

with $\varepsilon_{\sigma}^{(i)}(k_{||})$ denoting the creation (annihilation) operator for site $i$ and orbital $\sigma$. $\varepsilon_{\sigma}^{(i)}(k_{||})$ and $\varepsilon_{\sigma}^{(i)}(k_{||})$, respectively, are onsite and hopping matrix elements. The semi-infinite GaAs “leads” are taken into account by evaluating the associated self-energies and feeding them into the system’s Dyson equation. The surface Green’s functions are obtained with the help of an algorithm suggested by Sancho et al.

For each carrier type (majority and minority), the transmission function $T(E, k_{||})$ for total energy $E$ and in-plane momentum $k_{||}$ is calculated via

$$T(E, k_{||}) = \text{Tr} \left[ \Gamma_R G^R \Gamma_L G^A \right].$$

Here, $G^{R/A}$ are the system’s retarded (R) and advanced (A) Green’s functions, $\Gamma_{L/R}$ are the coupling functions to the left (L) and right (R) GaAs leads and $\text{Tr} [\cdot]$ is the trace operation. We then compute the steady-state current $j(V_a)$ assuming local thermal equilibrium among the electrons injected from a particular contact using the standard expression from stationary scattering theory

$$j(V_a) = \frac{2e}{h} \sum_{k_{||}} \int dE \left( T(E, k_{||}) f_L(E) - f_R(E) \right).$$
with e, ℏ, and $f_{L/R}$ denoting, respectively, the elementary charge, Planck’s constant, and the Fermi-Dirac distribution function for the left and right electric contacts. The applied voltage $V_a$ enters Eq. (6) in two places: the transmission function $T(E, k)$ and the difference in the quasi-Fermi levels between left and right contacts. In order to cut computational cost, we assume a linear voltage drop from the left to the right lead across the simulated structure. This implies a somewhat artificial relationship between the electric field across the structure and the applied bias.\textsuperscript{58,59} In principle, both an effective single-particle potential, an effective exchange splitting, and a self-consistent treatment of charge injection can be implemented into the present model.\textsuperscript{49} However, while providing a significant reduction in computation time, omission of self-consistency may not significantly reduce the quality of our results. Note that the Fermi-Dirac distributions of the GaAs contacts provide the sole temperature dependence in the current model since a temperature dependence of the electronic structure is not considered here. For a discussion of the latter, we refer to recent work.\textsuperscript{29}

In what follows we present results for the I–V characteristics of GaAs/(CrAs)$_{10}$/GaAs heterostructures for $\ell = 4, 6, 8, 10$. While thin layers of ZB CrAs may be easier to realize experimentally, thicker layers thereof are described more realistically within our approach. The free carrier density in the n-doped GaAs regions is about $4.5 \times 10^{17}$ cm$^{-3}$ at $T = 300$ K ($7.9 \times 10^{16}$ cm$^{-3}$ at $T = 0$ K), with the quasi-Fermi level held constant at 10 meV above the conduction band edge. The applied bias was varied between zero and 0.2 V. Results for scissored and un-scissored GaAs, respectively, and $\ell = 10$ are shown in Figs. 10 and 11 (mind the semi-logarithmic plot). The upper and lower curves of each pair correspond to majority and minority current density contributions, respectively. The overall features of the I–V characteristics agree for both cases: the majority current density clearly dominates over the minority current density and this, in most bias regions, by several orders of magnitude. However, spin-filtering is more pronounced for the scissored GaAs model. While the majority current is rather insensitive to scissoring, the minority current density is not (we believe that the small oscillations for the 77 K minority case near 1.5 V in Fig. 10 are of numerical origin). The reason is found by inspection of Figs. 1 and 2. It shows that, for un-scissored GaAs and low applied bias, there is a resonance between the GaAs conduction band minimum (dashed line) and CrAs-associated bands near the $\Gamma$-point. Near the $\Gamma$-point, these bands are rather flat and so the group velocity is almost zero. Under moderate bias, however, these bands are moved further into resonance (to regions with higher group velocity) with the conduction band of GaAs at the emitter side, and the minority current rises steeply with applied bias.

The current spin polarization $P(V_a)$ as a function of applied voltage $V_a$ is defined as
Here, $j_{\text{maj/min}}$ refers to the majority and minority spin current density, respectively. In Figs. 12 and 13, respectively, we display the computed current spin polarization for scissored and un-scissored GaAs and the three different temperatures discussed above.

In Fig. 14, we show the I–V characteristics as obtained for different layers thicknesses, i.e., $(\text{GaAs})_m/\text{(CrAs)}_\ell/(\text{GaAs})_m$, where $\ell = 4, 6, 8, 10$ and $m = 5$. The results shown in Fig. 14 stem from simulations in which the number of layers of GaAs to the left and the right of CrAs was set to $m=5$ and kept constant, i.e., the electric field across the CrAs layer at a given voltage increases with decreasing layer thickness. This trend follows the actual physical trend within the device and that of a self-consistent model. Moreover, we note that the actual form of the computed I–V characteristic is only slightly changed if our simulations are performed under equal-electric-field conditions, i.e., $m = 10 - \frac{\ell}{2}$ because the form of the bands involved in the transport of majority carriers (determining their transmission coefficient) is very robust under a slight change of the energy offset, see Figs. 6 and 7.

From Fig. 14, we clearly observe non-Ohmic behavior which is due to the rather complicated electronic structure involved in the transmission probability. We observe, for instance, that the absolute value of the current transmitted through a structure consisting of six layers CrAs is higher for all voltages than when transmitted through four layers. These I–V characteristics indicate that spin-filtering should also be realizable with very thin structures of CrAs, see Fig. 15, which might be easier to fabricate. For $n = 4$, the minority current shows nonlinearities, which we attribute to resonant transport mediated by states which, in the bulk, give rise to the bands discussed above. Nevertheless, it has to be kept in mind that the systematic error of our approach is larger for very thin structures because (i) the modeling of the CrAs layers is based on the Hamiltonian of bulk ZB CrAs and (ii) effects from the interface will become more important for thin layers. Nevertheless, spin-filtering should be observable.

V. SUMMARY, DISCUSSION, CONCLUSIONS, AND OUTLOOK

We have performed a model study of transport in CrAs/GaAs heterostructures, which is based on the assumption that sufficiently thin layers of CrAs can be grown in between a GaAs substrate in lattice matched fashion. The bulk electronic structure of (zinc-blende) bulk GaAs, zincblende and tetragonal CrAs, as well as lattice matched single [1,0,0] GaAs/CrAs heterointerfaces were calculated within an LSDA LMTO model and used to determine the band offsets between the two materials for minority and majority carriers. As a remarkable result, we find a (local) total energy minimum for a tetragonal bulk CrAs unit cell, when the transverse lattice constant is held fixed at the bulk GaAs value $a_{\text{GaAs}} = 5.65$ Å and the longitudinal [1,0,0] lattice $a_\perp$ constant is varied. The minimum is found for $a_\perp \approx 0.98 a_{\text{GaAs}}$. Although this local equilibrium unit cell of CrAs is tetragonal...
rather than cubic, the systematic errors introduced by assuming a perfectly lattice matched zinc-blende crystal structure at $a_{\text{GaAs}}$ are found to be negligible. For a lattice constant of $a_{\text{CrAs}} = 5.65$ Å, we find that zinc-blende CrAs is a half-metal, with zero gap for one spin orientation (majority carriers) and a gap of 1.8 eV at the X point for the other (minority carriers). The computed band offset for a lattice matched [1,0,0] hetero-interface between the two materials is found to be about 0.5–0.6 ± 0.2 eV. The latter implies an alignment of the gap region of minority CrAs with the central region of the uppermost valence bands of GaAs. For spin-filtering, therefore, it is not important whether the sheet of CrAs is half-metallic or not. The latter is important because theoretical studies have implied that the occurrence of half-metallicity in CrAs/GaAs superlattices is sensitive to layer thickness and lattice constant.

The ab-initio spin-dependent electronic band structures are mapped onto an ETB model, which is used to construct the effective Hamiltonian of the n-GaAs/CrAs/n-GaAs heterostructures consisting, respectively, of $\ell = 4, 6, 8, 10$ monolayers of CrAs. This down-folding was constrained by the requirement that As ETB onsite parameters for a given spin orientation be constant throughout the system, thereby, eliminating the need for the introduction of ad-hoc ETB parameters at the heterointerface. The non-linear current response for majority and minority carriers is obtained within a non-equilibrium Green’s function approach. We consider carrier injection from n-doped GaAs and our calculations show efficient spin-filtering over a wide parameter range, in particular, regarding the precise band alignment between the GaAs conduction band edge with the CrAs bands, temperature, and layer thickness. Spin-polarization of up to 99%, as well as room-temperature spin-filtering, is predicted within this model.

A number of potential improvements to the present theoretical approach, such as a more realistic account of correlations, a self-consistent treatment of non-linear transport, a more detailed inclusion of the interface, scattering, etc., can readily be listed and be addressed in future studies. We note that a recent GW study of ZB CrAs, MnAs, and MnC has revealed a rather insignificant change in the electronic structure and strained zinc-blende MnAs quantum dots on GaAs, the growth in the zinc-blende or tetragonal phase apparently has not been successful. Evidence for zinc-blende (or tetragonal) CrAs layers on GaAs substrates still seems to be controversial. It is hoped that these promising theoretical results regarding the CrAs electronic structure, the favorable band alignment with GaAs, and the high spin-polarization predicted in our non-linear charge transport calculations encourage the material growth and experimental physics community in a continued quest for transition metal compounds in the cubic structure and the study of semiconductor heterostructures containing them.

**ACKNOWLEDGMENTS**

The authors thank R. Hammer, M. Aichhorn, and E. Arrigoni for fruitful discussions. This work was supported financially by FWF Project No. P221290-N16.

**APPENDIX: TIGHT-BINDING PARAMETERS**

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<tr>
<th>$E_{s\sigma}$</th>
<th>CrAs maj</th>
<th>GaAs maj (A)</th>
<th>GaAs maj (B)</th>
<th>CrAs min</th>
<th>GaAs min (C)</th>
<th>GaAs min (D)</th>
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<tr>
<td>$E_{x\uparrow}$</td>
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<td>2.6574</td>
<td>2.6574</td>
<td>4.5703</td>
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<td>1.2291</td>
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<td>7.4409</td>
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TABLE I. Tight-binding parameters for bulk CrAs majority and minority spin and the respective GaAs parameters. The anion onsite energies are indicated by the number 1, while the cation is labeled by the number 2. For further notations, see Ref. 45.