

Orthogonal and Non-Orthogonal Tight Binding Parameters for III–V Semiconductors Nitrides

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Received: 6 July 2016 / Published online: 25 August 2016
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Abstract A simulated annealing (SA) approach is employed in the determination of different tight binding (TB) sets of parameters for the nitride semiconductors AlN, GaN and InN, as well their limitations and potentialities are also discussed. Two kinds of atomic basis set are considered: (i) the orthogonal sp^3s^* with interaction up to second neighbors and (ii) a spd non-orthogonal set, with the Hamiltonian matrix elements calculated within the Extended Hückel Theory (EHT) prescriptions. For the non-orthogonal method, TB parameters are given for both zincblend and wurtzite crystalline structures.

Keywords Electronic structure · III-V nitrides · Tight-binding · Band structure · Monte Carlo

1 Introduction

Even nowadays, semiconductor systems are widely studied experimentally and theoretically due to their broad application in optoelectronics. Despite the huge technological growth of red and yellow light-emitting diodes (LEDs), there are still efforts to extend their operation into the short wavelength region of the visible spectrum (from green to violet). Although successful attempts to make LEDs and LDs with SiC and II-VI materials (e.g., ZnSe) have been made, the purpose of such devices has been diminished by

the very low efficiency in SiC diodes and the short lifetimes of carriers in II–VI materials, which is due to the relative facility of defect formation. As a result, the III–V nitride materials with wurtzite crystal structure (GaN, AlN, InN, and their alloys) have generated considerable interest for operation at these short wavelengths. Since the electronic band structure for each one of the nitride materials possesses a direct transition with a band gap energy range from 1.9 eV (InN) to 6.2 eV for AlN at room temperature as well rather high thermal conductivity, the (AlIn)GaN system has been explored in the areas of high-power and high-temperature electronic devices and short-wavelength (visible and ultraviolet) optoelectronic devices. See [1, 10] for a review of relevant properties of these compounds.

It is known that semiconductor devices and nanostructures simulations demand large supercells, requiring a great computational effort if the systems properties are calculated within first-principle approaches. On the other hand, the theoretical description of large supercells is possible within the semi-empirical tight-binding (TB) formalism with modest computational load. TB calculations employ atomic orbitals as basis set, with the Hamiltonian matrix elements (orbital energies and hoppings) being parameterized in order to reproduce the experimental band structure of the crystalline material. The basis of the TB method applied to Solid State Physics were established in the seminal paper of Slater and Koster [3], which assumes the atomic orbitals as an orthogonal basis set: the so called Orthogonal Tight Binding (OTB) formalism. The TB parameters in the orthogonal formulation have reduced their transferability for different environments from the ideal crystalline structure they were first calculated. For instance, the description of pressure effects on the electronic properties of crystals is only possible with a suitable correction of the hopping elements, which are due the atom-atom distance reduction.

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One alternative to OTB is to approach the problem within the semi-empirical Extended Hückel Theory (EHT) [4, 5]. As in any TB formalism, the EHT alloy states are spanned as linear combinations of atomic orbitals, considering that the basis orbitals form a non-orthogonal basis set. The aforementioned method presents a good transferability of its parameters [4], and it also gives a good description of the deformation potential for III–V alloys under uniform strain [5]. In addition, EHT is capable of reproducing the density of states (DOS) of graphene, silicene, and germanene supercells with a single vacancy, in a remarkable agreement with Density Functional Theory (DFT) calculations [6].

The paper is organized as follows. In Section 2, a summary of the theoretical tools employed for studying the alloys is presented, namely the tight binding approach for the electronic structure calculations in both orthogonal and non-orthogonal (Hückel) formulation and the Simulated Annealing (SA) method for calculating the TB parameters. Finally, Section 5 presents all the TB sets in both orthogonal and non-orthogonal formulations and a discussion about the quality of the sets, measured in terms of few physical parameters: root mean square (RMS) deviation of the TB bands from the target bands, the resulting TB electronic gaps and effective masses.

2 III-V Nitrides: Band Gaps and Structural Properties

AlN, GaN, and InN nitrides are wide-gap semiconductors that usually crystallize in the wurtzite (WZ) lattice. However, under certain conditions, the zincblende (ZB) crystal structure can be obtained by growing the materials on zincblende substrates. Table 1 resumes their structural parameters and gaps at Γ . All these compounds, except AlN in ZB structure, are direct gap and their alloys as well their quantum wells are important from the application perspectives such as optoelectronics, because these compounds are the key constituent in blue diode lasers and LEDs [10] active regions.

The zincblende crystal structure consists in two interpenetrating face centered cubic (FCC) lattices, where each sublattice is occupied by a different chemical specie. There are

two atoms/unit cell in a FCC structure: One is located at the origin and the other at $a(1/4, 1/4, 1/4)$ position, where a is the lattice parameter. The wurtzite unit cell has hexagonal symmetry and its unit cell has four basis atoms occupying the following positions: the N anions at $(a/3, 2a/3, 0)$ and $(2a/3, a/3, c/2)$, and the N cations at $(a/3, 2a/3, 3c/8)$ and $(2a/3, a/3, 7c/8)$.

3 Formalism

3.1 Orthogonal Tight-Binding Formalism

The description of the electronic structure within the OTB is given in the seminal paper by Slater and Koster [3]. Within the two center approximation, it is assumed the basis orbital forms an orthogonal set, and the Hamiltonian matrix elements between two basis orbitals are expressed only in terms of the orbital's symmetry and the distance among them, not considering the contributions from atoms localized in different lattice sites. The inclusion of d orbitals in the basis is needed for a good description of the bands, but increases the computational effort. On the other hand, a device first introduced by Vogl [2] consists in replacing the 5 d orbitals for an effective excited s orbital, s^* . Thus, it is employed a sp^3s^* basis for the TB description of the electronic structure in the orthogonal formulation, avoiding this way the use of d orbitals.

Within the sp^3s^* basis, the TB bulk Hamiltonian is written as

$$H = \sum_{ij\mu\nu} h_{ij}^{\mu\nu} c_{i\mu}^\dagger c_{j\nu} \quad (1)$$

where i and j denote the sites in the zincblende structure and μ and ν denote the atomic orbitals. The spin-orbit corrections are neglected in the parameter calculations. The $h_{ij}^{\mu\nu}$ values in 1 correspond to all the on-site orbital energies ($i = j$) and hoppings ($i \neq j$). In this article, the hoppings $h_{ij}^{\mu\nu}$ for AlN, GaN, and InN compounds are restricted to pairs (i, j) up to second neighbors, yielding in two kind of TB sets. Within this approach, the band structure is calculated by diagonalizing the 10×10 Hamiltonian built in the

Table 1 Structural properties and gaps of the Nitride binary compounds studied in this article

Compound	a (zincblend)	a, c (wurtzite)	E_{gap} (zincblend)	E_{gap} (wurtzite)
GaN	4.50	$a = 3.19$ $c = 5.18$	3.30	3.51
AlN	4.38	$a = 3.11$ $c = 4.98$	4.90	6.23
InN	4.98	$a = 3.54$ $c = 5.70$	1.94	1.99

basis of Bloch sums of the corresponding atomic valence orbitals.

3.2 The Extended Hückel Theory

The EHT calculations shares with other Tight-Binding approaches the use of atomic orbitals as basis sets, but in comparison with the OTB formulation, the method works with explicit analytical expressions for the basis orbitals. As a result, a price to be paid is the additional calculation of the overlap matrix **S** among the basis orbitals. A common choice is to express the basis orbitals { Φ_ν } as a sum of two Slater-Type Orbitals (STO) (double zeta basis). The matrix elements of the Hamiltonian in the EHT in terms of the atomic basis set are:

$$\begin{aligned}
 H_{\mu\mu} &= \langle \Phi_\nu | H | \Phi_\nu \rangle = E_{\mu\mu} \\
 H_{\mu\nu} &= \frac{1}{2} K_{\text{EHT}} (H_{\mu\mu} + H_{\nu\nu}) S_{\mu\nu} \\
 S_{\mu\nu} &= \langle \Phi_\mu | \Phi_\nu \rangle = \int \phi_\mu^* \phi_\nu d^3 \mathbf{r},
 \end{aligned}
 \tag{2}$$

where K_{EHT} is an additional fitting parameter whose value is commonly set to 1.75 for molecules and 2.3 for solids [4], and $S_{\mu\nu}$ is the overlap between the $|\Phi_\mu\rangle$ and $|\Phi_\nu\rangle$ orbitals. In order to perform calculations within the EHT, it is necessary to specify, for each atom type, the onsite energies (E_s , E_p , and E_d), the zetas of the Slater Orbitals, and the first expansion coefficient c_1 . The second coefficient value is constrained in order to guarantee the orbital normalization. The Tight-Binding band structure is obtained by solving the generalized eigenvalue problem:

$$\mathbf{H}(\mathbf{k})\Psi_i(\mathbf{k}) = E_i(\mathbf{k})\mathbf{S}(\mathbf{k})\Psi_i(\mathbf{k}),
 \tag{3}$$

where $\Psi_i(\mathbf{k})$ denotes the eigenvector of the i th band, and \mathbf{k} is the Bloch wave vector within the first Brillouin Zone. The overlap and Hamiltonian matrices, $S(\mathbf{k})$ and $H(\mathbf{k})$, are calculated through

$$H_{i,j}(\mathbf{k}) = \sum_{j',m'} e^{i\mathbf{k}\cdot(\mathbf{R}_{i0}-\mathbf{R}_{j'm'})} H_{i0,j'm'}
 \tag{4}$$

$$S_{i,j}(\mathbf{k}) = \sum_{j',m'} e^{i\mathbf{k}\cdot(\mathbf{R}_{i0}-\mathbf{R}_{j'm'})} S_{i0,j'm'},
 \tag{5}$$

Table 2 OTB sets for both 1nn and 2nn models. The top of the valence band for all compounds was set to zero

	AlN		GaN		InN	
	1nn	2nn	1nn	2nn	1nn	2nn
E_{sa}	-4.1253	-4.7340	-2.9928	-6.9892	-12.0165	-3.2307
E_{pa}	0.2013	-0.2575	8.2421	0.0087	5.2396	2.0365
E_{sta}	21.1872	26.3273	7.4040	28.5516	7.5473	25.1512
E_{sc}	-3.5695	0.3229	-9.1457	-1.1585	-0.0208	-2.1405
E_{pc}	20.3600	11.2192	18.5207	10.0413	15.4685	7.8761
E_{stc}	14.7917	20.3649	24.7712	18.8317	14.4429	22.3537
V_{ss}	-10.6435	-9.4920	-9.0571	-8.4367	-5.5534	-8.0127
V_{xx}	2.2916	3.2124	12.2267	3.2616	8.9166	6.1282
V_{xy}	6.2680	4.7497	15.0712	5.9180	11.3494	6.4427
V_{sapc}	5.2908	3.9682	8.9932	1.7631	3.4244	4.9504
V_{pasc}	10.8227	12.1895	8.8691	12.0073	7.3719	12.0874
V_{stapc}	16.4151	7.4956	6.6838	6.7579	4.9810	8.1301
V_{pastc}	0.4568	0.0001	0.4338	0.0002	3.2377	0.0002
V_{stst}	0.2000	0.0000	0.1313	0.0000	0.0216	0.0000
V_{sasa}		-1.4466		-1.2606		-1.6509
V_{sxa110}		0.7521		0.9329		1.0310
$V_{stxa110}$		-0.0144		-0.0793		-0.0001
V_{xxa110}		0.4155		0.3533		0.5828
V_{xxa011}		-0.0089		-0.0020		0.0355
V_{xya110}		1.0982		0.9027		1.2079
V_{scsc}		-0.1839		-0.1811		-0.7139
V_{sxc110}		1.1282		0.9257		0.8519
$V_{stxc110}$		-0.0071		-0.0157		-0.0170
V_{xxc110}		2.7809		1.9169		1.6969
V_{xxc011}		-0.1486		-0.0858		-0.0263
V_{xyc110}		0.3100		0.6717		1.3816

Table 3 Optimized parameters of the atomic orbitals (AO) basis set calculated by SA

	AO	ζ_1	c_1	ζ_2	$c_2=$
N	2s	2.4161	0.9399		
	2p	1.8569	0.9221	3.4019	0.3870
	3d	0.7243	0.4181		
Al	3s	1.5943	0.6926		
	3p	1.1362	0.6200	4.5546	0.7846
	3d	0.7423	0.6570	4.6871	0.7539
Ga	4s	2.0033	0.6356		
	4p	1.6068	0.7761	8.9752	0.6307
	4d	1.0399	0.6364		
In	5s	2.3211	0.7212		
	5p	1.9476	0.7325	8.4423	0.6808
	5d	1.3491	0.6423		

Although all AO's are of the double- ζ Slater type, the values of the c_2 coefficient are not included whenever $\zeta_2 = 25$ and, for these cases, $c_2 = \sqrt{1 - c_1^2}$. The K value in (2) was set to 2.3 and the Fermi Level was fixed to -13 eV

where i and j label the atoms within the unit cell and m' is the unit cell index. The summation indices in (4) and (5) run over all atoms j' in the unit cell m' which are equivalent to atom j in the reference unit cell $m = 0$. The real-space matrix elements $H_{i0,j'm'}$ and $S_{i0,j'm'}$ constructed between an atom i in the reference unit cell and atom j' in cell m' are calculated through the Extended Hückel prescription (2). In addition, hoppings were restricted to sites with inter-atomic distances less than 9 \AA (cutoff radius).

4 Simulation Annealing Procedure

As published in [5], all TB parameters were calculated using a simulated annealing (SA) approach within the proposal of Vanderbilt and Louie [7]. In a few words, for a given initial set of Hückel parameters, their values are varied in

Table 5 Final values of the RMS for all TB models

Compound	Zincblend			Wurtzite
	OTB 1nn	OTB 2nn	Hückel	Hückel
AlN	0.540	0.096	0.096	0.099
GaN	0.312	0.071	0.129	0.068
InN	0.229	0.095	0.135	0.102

successive Monte Carlo cycles with decreasing temperatures in order to reduce the value of the objective function y , namely the root mean square (RMS) deviation of the Hückel bands $E_i^H(\mathbf{k})$ in relation to a target band structure $E_i^T(\mathbf{k})$:

$$y = \sqrt{\frac{1}{nb \times nk} \sum_{i=1}^{nb} \sum_{j=1}^{nk} [E_i^H(\mathbf{k}_j) - E_i^T(\mathbf{k}_j)]^2}, \quad (6)$$

where nb and nk denote, respectively, the number of bands and k -points. The target band structure was calculated by the *ab-initio* Density Functional Theory (DFT) formalism as implemented in the Abinit package [8], with plane wave cutoff energy of 40 Ha and Hartwigsen-Goedecker-Hutter pseudopotentials [9]. The calculations were carried out using the Generalized Gradient Approximation (GGA) as parameterization of the exchange-correlation potential and the bands were generated along the $\Gamma - X - L - \Gamma$ lines for the zincblend structure and $M - L - A - \Gamma - K - H$ for the wurtzite.

As DFT underestimates the band gap value, its conduction bands were shifted by the difference between the experimental and the DFT gap values. In the minimization procedure, all valence bands and the first conduction bands were included in (6). An acceptable set is generated when $y \leq 0.15$ eV. This approach was successful for generating acceptable and highly transferable TB sets for few III–V semiconductors compounds (AlAs, GaAs, InAs, and GaP) [5], as well and group IV planar structures such as graphene, silicene and germanene [6].

Table 4 Optimized atomic basis orbitals on-site energies for both zincblend and wurtzite crystalline structures

Compound	Element	Zincblend			Wurtzite		
		E_s	E_p	E_d	E_s	E_p	E_d
AlN	Al	-12.9281	-8.6090	-4.4930	-12.7164	-8.0662	-4.8278
	N	-23.5307	-13.4971	-2.5044	-23.7799	-13.6877	-2.1462
GaN	Ga	-15.6698	-8.7221	-3.8077	-15.5754	-9.1129	-3.4400
	N	-23.8265	-13.4739	-3.0276	-23.6683	-13.4821	-3.7490
InN	In	-15.0021	-8.7243	-1.5326	-14.9593	-8.8241	-1.4675
	N	-23.7727	-13.0180	-1.0627	-23.7213	-13.0377	-0.8192

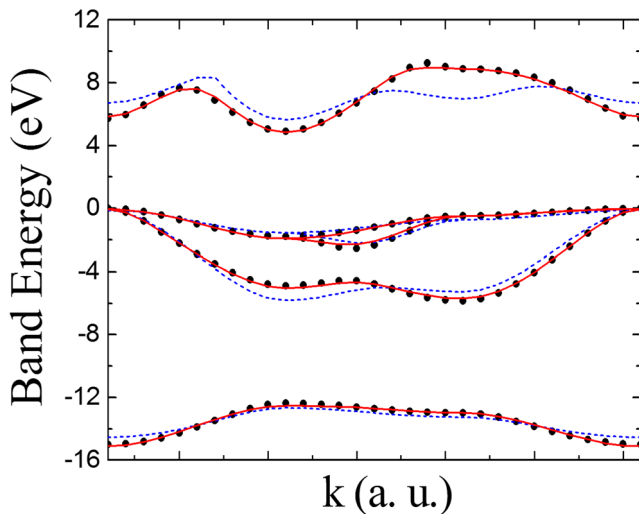


Fig. 1 Comparison of the resulting bands for the 1nn (blue dashed) and 2nn TB sets with respect to the target DFT bands (dots)

5 Results and Discussion

5.1 OTB parameters

As two orthogonal TB sets are presented for each compound, one set has only first-neighbor hoppings and the other set has hoppings up to second neighbors, let's denote them, respectively, as OTB 1nn and OTB 2nn. For a given zincblend compound, the TB parameters in the OTB formulation can be divided in two groups: one referring to the anion atom (*a*) and other to the cation (*c*). For the sp^3s^* basis set, the OTB parameters correspond to the onsite energies values for the anions (E_{sa} , E_{pa} , and E_{sta}) and for the cations (E_{sc} , E_{pc} , and E_{stc}) and the first neighbor hoppings (V_{ss} , V_{xx} , V_{xy} , V_{sabc} , V_{pasc} , V_{stapc} , V_{pastc} , V_{sst} , and V_{stst}) and the corresponding second neighbor hoppings. In order to reduce the number of parameters to be fitted, for all OTB 1nn sets it is assumed $V_{sst} = 0$ and $V_{ssta} = V_{sstc} = V_{ststa} = V_{ststc} = 0$ (Table 2).

5.2 Hückel Parameters

The optimized set of parameters for GaN, AlN, and InN compounds are summarized in Tables 3 and 4. In the SA procedure, all valence bands and the first conduction band were included, resulting a total of five bands for zincblend

and nine for wurtzite structures. The systematic adopted in SA procedure was first optimize the AlN, and for GaN and InN, the values of ζ and c_1 of N were set to the calculated values for AlN, emphasizing only orbital energies for this specie are varied.

As the parameters for GaN were already calculated in [5], in this paper, the parameters were recalculated. In Table 4, the onsite energies are given for both zincblend and wurtzite structures. The parameters were generated first for the zincblend structure; moreover, in order to test their transferability, only the onsite energies were varied in the parameterization procedure for the wurtzite structure. As previously published in [5] for other III–V compounds, the atomic orbital related parameters depend only on the atomic specie, being the same for both zincblend and wurtzite. For all compounds, the final RMS value was always less than 0.16, with the worst value obtained for InN. The onsite energies follow the same trend: as lighter the element, more close are the values for the wurtzite onsite energies with respect to zincblend.

From Table 4, it is possible to assess the parameters transferability and even the small impact of the crystalline environment on the onsite energies. For the AlN and GaN, better RMS values were obtained and even for the InN, it is possible to assert the quality of the parameters by the following way: the wurtzite unit cell has four atoms, and for this structures, the minimization procedure was carried out just considering a number of valence bands twice compared to the zincblend structures, whose unit cell has two atoms.

5.3 Discussion

In Table 5, there is a summary of the final RMS values for all calculated sets by the SA method. As expected, the best parametrizations correspond to the OTB 2nn and the one given by the Hückel model. Figure 1 shows the calculated band structures of AlN for the 1nn and 2nn OTB models compared to the target DFT bands. AlN was choose because its the 1nn model result the worst RMS value of Table 5, whereas the other models yield excellent fits. As the value of the final RMS for the Hückel set is very close to the 2nn model, the corresponding bands were not included in the Fig. 1 in order not to overload it. Notice that in the figure, the excellent overall agreement of the 2nn model with the DFT bands and an acceptable for the valence bands of the

Table 6 Calculated gaps in eV for all models considered

Compound	Zincblend				Wurtzite	
	Target	OTB 1nn	OTB 2nn	Hückel	Target	Hückel
AlN	4.90	5.74	4.88	4.86	6.23	6.21
GaN	3.30	3.38	3.40	3.12	3.51	3.43
InN	1.94	2.18	2.22	2.07	1.99	2.11

Table 7 Calculated effective masses for all models and compounds (zincblend)

	Compound	Zincblend			
		Target	OTB 1nn	OTB 2nn	Hückel
$m_e(\Gamma)$	AlN	0.25	0.742	0.378	0.369
	GaN	0.15	0.188	0.215	0.192
	InN	0.12	0.133	0.140	0.152
$m_l(X)$	AlN	0.53	0.463	0.451	0.617
	GaN	0.5	2.68	0.546	0.694
	InN	0.48	2.735	1.643	1.416
$m_t(X)$	AlN	0.31	0.467	0.388	0.312
	GaN	0.3	0.342	0.296	0.264
	InN	0.27	0.308	0.288	0.304

1nn model; furthermore, even the 1nn model gives a bad description of the conduction band, the description of the region around the minimum is not so bad.

Aiming to quantify the quality of all TB sets, Tables 6 and 7 present, respectively, the calculated gaps and the effective mass of all compounds in the zincblend structure. Regarding the gaps, the calculated values for all TB models show deviations less than 5 % from the corresponding target values. For the effective masses, the deviations for the best models were less than 45 % and this result is acceptable, because the fit procedure adopted in this work do not use the effective masses as target values, as the TB parameters fitted by Klimeck and collaborators [11, 12] for some group IV and III-V semiconductors.

As expected, the OTB 2nn and the Hückel model result in a better description of the effective masses, although the 1nn model does gives non pathological values for the $m_e(\Gamma)$ and $m_t(X)$ masses. However, for all models, the $m_l(X)$ for InN is very high compared to the target value. In this case, there is an interesting feature of the present proposal: the effective masses values reflect the quality of the target band structure, and as better were the target bands better will be the values of the calculated effective masses. The so called band gap problem in the DFT calculations was overcome by adding the difference between the experimental and the DFT gap values; however, for the effective masses, there is no similar device because the values of the effective masses will depend on the correct description of the curvature bands around the edge. In the present case, the target bands were calculated within the standard DFT calculations employing the GGA approximation for the exchange-correlation potential. However, a even more precise calculation can be done within the state-of-art quasiparticle calculation based on the GW approximation [13].

There are few TB parameters published in the literature for the compounds considered here. In the work of

Gürel and collaborators [14], the authors use sp^3s^* basis set with orbital interaction up to second neighbors, but only the hoppings between second neighbors p orbitals are considered, all the others being set to zero. However, the authors in the paper not present a comparison between the resulting bands with bands calculated with other methods: just the energies in the high-symmetry points of the BZ are presented. On the other hand, in the paper of Jancu et al. [15], a $sp^3d^5s^*$ basis set is employed, with only nearest-neighbor orbital interaction. This article presents TB sets for both zincblend and wurtzite phases and the exponents of the Harrison scaling Law for the hoppings, needed for correct them in the case of deviation of the atomic position from the ideal crystal values. Thus, despite the use of d orbitals, the calculated bands and the effective masses are well described in this model, being this paper a reference for TB sets for the AlN, GaN, and InN compounds.

Concerning the Hückel parameters, this article publish the first parametrization for the AlN and InN compounds in both zincblend and wurtzite crystalline structures. Different from the OTB sets, which need the exponents of the Harrison scaling Law for correcting the hoppings when the system suffers structural deformations, the Hückel parameters are highly transferable. Moreover, being the hoppings proportional to the overlap between the involved orbitals, their values are corrected just recalculating the overlap and this is a great advantage of the EHT over OTB.

6 Conclusions

The article presents a Simulated Annealing approach for calculation of the TB parameters for the group III nitrides AlN, GaN, and InN. The sets are divided in two “flavors”: orthogonal basis set (OTB) and Hückel non-orthogonal parameters. For the former, both nearest and second nearest

neighbor sets are presented for a sp^3s^* basis and zincblend structure and, for the later, the Hückel parameters were calculated in for a spd basis and for both zincblend and wurtzite phases.

Acknowledgments The author is grateful for the financial support of the Brazilian funding agency Fundação de Amparo à Pesquisa do Estado do Rio de Janeiro (FAPERJ) through grants E-26/112.554/2012 and E-26/110.318/2014. The author also would like to thanks to I. A. Ribeiro for the kind revision of the manuscript.

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