TCAD Parameters for 4H-SiC: A Review

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In this paper we review the models and their parameters to describe the relative permittivity, bandgap, impact ionization, mobility, charge carrier recombination/effective masses and incomplete dopant ionization of 4H silicon carbide in computer simulations. We aim to lower the entrance barrier for newcomers and provide a critical evaluation of the status quo to identify shortcomings and guide future research. The review reveals a rich set of often diverging values in literature based on a variety of calculation and measurement methods. Although research for all the selected parameters is still active, we show that sometimes old values or those determined for other kinds of silicon carbide are commonly used.

Keywords: 4H-SiC, TCAD simulations, simulation parameters, silicon carbide

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I. BAND GAP

The band diagram of a material specifies the energy of a charge carrier for a given direction-dependent momentum. The electrons are described by the *conduction band* and the holes by the *valence band*. If both touch the material is called a conductor while a large gap, called the *band gap*, characterizes an insulator. Materials having a band gap in between these two extremes are called semiconductors. This shows that an exact knowledge of the band gap is instrumental to describe the electronic properties of 4H-SiC.

In TCAD simulations the band gap E_g is essential for the carrier concentration, in the drift diffusion equation and also for the barrier heights in Schottky contacts. Because E_g is often stated in the exponent, where small changes can have a huge impact, a high accuracy is desired. In this section we are, thus, going to investigate band gap energies published in literature by extending existing overviews[1,2]. Overall, we conclude that the majority of the currently used values are, with high confidence, based on measurement from the year 1964. Despite various variations and changes the most commonly used value coincidentally fits latest measurements, however further investigations are required for proper confirmation.

A. Theory

The band gap is measured between the highest energy value of the valence band in the Γ point (see **??**) and the lowest one of the conduction band in the M-point[3–5]. Because these are not at the same location 4H-SiC is a so-called indirect semiconductor, which means that some transfer of moment, e.g., by a phonon, is required for the minimum energy difference. Electrons can also be lifted from the valence to the conduction band in the Γ point and then gradually relax towards the minimum, however, in that case more than the band gap energy is required to create an electron-hole pair. An overview of ionization energies for these cases is provided by Gsponer *et al.* [6], who extracted a value of (7.83 ± 0.02) eV from their own measurements.

Our statement that electrons are lifted from the valence to the conduction is not completely correct. Actually, the electron first forms an exciton by Coulomb interactions with the hole it left behind[7–10]. This setup can be compared to the hydrogen atom but with much larger radii due to the much lower effective masses. Additional energy has to be provided before the electron can move freely within the conduction band. Consequently, the band gap energy E_g is the sum of the

energy required to generate the exciton, i.e., the exciton band gap energy E_{gx}, and the energy to free the electron from the exciton, i.e., the *free exciton binding energy* E_x (see Eq. (1)[11]).

$$E_g = E_{gx} + E_x \tag{1}$$

The free exciton binding energy E_x must not be confused with the *bound* exciton binding energy[7,12–22]. An exciton, which is neutral and thus can relatively easily travel through the lattice, can achieve an energetically better configuration when attaching itself to an impurity[7]. The energy reduction relative to E_{gx} is represented by the bound exciton binding energy, which depends on the impurity atom, the lattice site and the charge state[23]. Typical values reported in literature are comparable to the free exciton binding energy (in the range of a few meV). Because the same symbol E_x is used it is challenging to distinguish bound and free exciton binding energy.

The band gap energy is not a constant. First and foremost it varies among the polytypes of silicon carbide. It was empirically shown that the band gap scales linearly with the degree of hexagonality, i.e., the ratio of hexagonal to cubic lattice sites[24–27]. Because 4H-SiC has a hexagonality of 50 %[28] (cp. **??**) its band gap energy is located halfway between the extreme values. In addition the band gap changes with pressure[29], under strain[30] and for varying temperature and doping concentrations. These have a significant effect on the device behaviour as the shift in the band edges create, for example, potential barriers which influence the carrier transport across junctions[31].

In the sequel we are going to investigate band gap narrowing described by Eq. (2), whereat $E_g(T)$ denotes the temperature induced variation and $\Delta E_g(N_D^+, N_A^-)$ the doping-induced one.

$$E_g(T, N_D^+, N_A^-) = E_g(T) - \Delta E_g(N_D^+, N_A^-) \tag{2}$$

1. Temperature Dependency

Lattice vibrations cause a shift of the band energies and changes in the electron-lattice interaction energy[32]. Because these changes differ among energy levels the effective band gap changes[33]. The temperature dependent band gap (see Eq. (3))[29] contains effects from thermal expansion ($\Delta E_{th}(T)$) and electron-phonon interaction ($\Delta E_{ph}(T)$).

$$E_g(T) = E_g(0) - \Delta E_{th}(T) - \Delta E_{ph}(T) \tag{3}$$

These effects are hard to separate in experiments[29], which was, so far, only achieved by Cheng, Yang, and Zheng[34]. Because $\Delta E_{\mathrm{th}}(T)$ has a much weaker impact[35] and the scaling of both contributions is comparable[36] the models for $\Delta E_{\mathrm{ph}}(T)$ are, in general, used to describe both with reasonable accuracy. Arvanitopoulos *et al.*[37] extended Eq. (3) by adding an additive term $\Delta_{\mathrm{g}}^{\mathrm{Fermi}}$ to account for carrier statistics. This is, however, only necessary for devices whose size is close to the de-Broglie wavelength.

For high temperatures the band gap decreases linearly[38–40] while for low temperatures non-linear behavior, i.e., quadratic[39] or plateau-like behavior[41] is observed. Quadratic behavior is described by the empirical Varshni relation in Eq. (4)[42] with T_{g} some arbitrary characterization temperature.

$$E_{\mathrm{g}}(T) = E_{\mathrm{g}}(T_{\mathrm{g}}) + \alpha \left(\frac{T_{\mathrm{g}}^2}{T_{\mathrm{g}} + \beta} - \frac{T^2}{T + \beta} \right) \tag{4}$$

Multiple authors[35,36,41] criticize that it is not possible to retrace the parameters of this model to physical mechanism-specific quantities (e.g., β was said to be approximately the Debye temperature which turned out to be not the case, since it sometimes even got negative[43–45]) and the model is unable to provide adequate interpretation of available data sets at low and high temperature[46,47]. For example, Pässler[47] tried to match the values from Choyke, Hamilton, and Patrick[24] but achieved only unrealistic results.

A physically based approach describing a plateau-like behavior at cryogenic temperature is a model of Bose-Einstein type in Eq. (5)[41,48] with Θ_{B} the mean frequency of the involved phonons and α_{B} the strength of the electron-phonon interaction[29].

$$E_{\mathrm{g}}(T) = E_{\mathrm{B}} - \alpha_{\mathrm{B}} \left(1 + \frac{2}{\mathrm{e}^{\Theta_{\mathrm{B}}/T} - 1} \right) \tag{5}$$

The rate of change of the band gap at low temperatures is strongly material specific and depends on the phonon dispersion Δ[47]. Eq. (4) is most accurate for $\Delta \gg 1$[39,49], while Eq. (5) represents the lower limit ($\Delta \rightarrow 0$) and is most suitable for $\Delta < \frac{1}{3}$[47]. Because most semiconductors show a dispersion in the range of 0.3–0.6[47] Pässler[35,47] proposed the model shown in Eq. (6) with ε the entropy and Θ_{p} the average phonon temperature.

$$\begin{aligned} E_{\mathrm{g}}(T) = & E_{\mathrm{g}}(0) - \frac{\varepsilon \Theta_{\mathrm{p}}}{2} \left[\sqrt[p]{1 + \left(\frac{2T}{\Theta_{\mathrm{p}}} \right)^p} - 1 \right] \\ p \approx & \sqrt{\frac{1}{\Delta^2} + 1} \end{aligned} \tag{6}$$

This model was subsequently extended by Pässler[39] to cover a wider range of the phonon dispersion Δ and, thus, promises to bridge the gap between Eq. (4) and Eq. (5).

2. *Doping Dependency*

The band gap also changes due to many-body effects of free carriers, i.e., their interactions among each other and with dopants, which become dominant for small carrier-to-carrier distances (high doping concentrations)[50]. Examples are interactions within a band, across bands and with ionized dopants[50–52]. The single effects were investigated extensively on their own[50] and got eventually merged, based on a similar analysis for silicon[51], for 4H-SiC by Lindefelt[52] to the model shown in Eq. (7).

$$
\begin{aligned}
\Delta E_{\mathrm{g}}(N_{\mathrm{D}}^{+},N_{\mathrm{A}}^{-}) &= -\Delta E_{(\mathrm{n/p})\mathrm{c}}(N_{\mathrm{D}}^{+}) + \Delta E_{(\mathrm{n/p})\mathrm{v}}(N_{\mathrm{A}}^{-}) \\
\Delta E_{\mathrm{nc}}(N_{\mathrm{D}}^{+}) &= A_{\mathrm{nc}}\left(\frac{N_{\mathrm{D}}^{+}}{10^{18}}\right)^{1/3} + B_{\mathrm{nc}}\left(\frac{N_{\mathrm{D}}^{+}}{10^{18}}\right)^{1/2} < 0 \\
\Delta E_{\mathrm{nv}}(N_{\mathrm{D}}^{+}) &= A_{\mathrm{nv}}\left(\frac{N_{\mathrm{D}}^{+}}{10^{18}}\right)^{1/4} + B_{\mathrm{nv}}\left(\frac{N_{\mathrm{D}}^{+}}{10^{18}}\right)^{1/2} > 0 \\
\Delta E_{\mathrm{pc}}(N_{\mathrm{D}}^{+}) &= A_{\mathrm{pc}}\left(\frac{N_{\mathrm{A}}^{-}}{10^{18}}\right)^{1/4} + B_{\mathrm{pc}}\left(\frac{N_{\mathrm{A}}^{-}}{10^{18}}\right)^{1/2} < 0 \\
\Delta E_{\mathrm{pv}}(N_{\mathrm{D}}^{+}) &= A_{\mathrm{pv}}\left(\frac{N_{\mathrm{A}}^{-}}{10^{18}}\right)^{1/3} + B_{\mathrm{pv}}\left(\frac{N_{\mathrm{A}}^{-}}{10^{18}}\right)^{1/2} + C_{\mathrm{pv}}\left(\frac{N_{\mathrm{A}}^{-}}{N_{\mathrm{A0}}}\right)^{1/4} > 0
\end{aligned}
\tag{7}
$$

ΔE_{nc} and ΔE_{pc} denote the change of the conduction band due to n and p type doping. Because the conduction band energy level drops these factors are negative and thus have to be subtracted from the increase of the valence band denoted by ΔE_{nv} and ΔE_{pv}.

The term featuring C_{pv} was added in an extension proposed by Persson, Lindefelt, and Sernelius[53]. The authors define the validity of this model for ionized charge carrier concentrations (see **??**) above a few $10^{18}\,\mathrm{cm}^{-3}$ and claim that a larger displacement is observable in 4H compared to other polytypes. More specifically, the valence band displacement is larger than the conduction band one. Other publications distribute the band gap narrowing equally across valence and conduction band[37] or chose a contribution of $\Delta E_{\mathrm{c}}/E_{\mathrm{g}} = 0.7$[54].

Some TCAD tools merge the prefactor and the denominator 10^{18} often called Jain-Roulston model[51], as shown in Eq. (8). We get $A_{x\mathrm{c}}^{\mathrm{j}}/A_{x\mathrm{c}} = 10^{-6}$ and $B_{xy}^{\mathrm{j}}/B_{xy} = 10^{-9}$ with $x \in \{\mathrm{n},\mathrm{p}\}, y \in \{\mathrm{c},\mathrm{v}\}$. For the remaining parameters the correlation is not so simply, i.e., we get $A_{x\mathrm{c}}^{\mathrm{j}}/A_{x\mathrm{c}} =\approx$

3.162×10^{-5}. For better comparison we transferred all parameters of Eq. (8) back to their respective counterparts in Eq. (7), except the sum of B_{xy}, which could obviously not be separated.

$$\begin{aligned}\Delta E_{\mathrm{gn}} &= -A^{\mathrm{j}}_{\mathrm{nc}}\left(N_{\mathrm{D}}^{+}\right)^{1/3} + \left(B^{\mathrm{j}}_{\mathrm{nv}} - B^{\mathrm{j}}_{\mathrm{nc}}\right)\left(N_{\mathrm{D}}^{+}\right)^{1/2} + A^{\mathrm{j}}_{\mathrm{nv}}\left(N_{\mathrm{D}}^{+}\right)^{1/4} \\ -\Delta E_{\mathrm{gp}} &= A^{\mathrm{j}}_{\mathrm{pc}}\left(N_{\mathrm{A}}^{-}\right)^{1/3} + \left(B^{\mathrm{j}}_{\mathrm{pv}} - B^{\mathrm{j}}_{\mathrm{pc}}\right)\left(N_{\mathrm{A}}^{-}\right)^{1/2} + A^{\mathrm{j}}_{\mathrm{pv}}\left(N_{\mathrm{A}}^{-}\right)^{1/4}\end{aligned} \tag{8}$$

An alternative approach to describe the doping dependency is to use the Slotboom model (see Eq. (9)), which was originally developed for Si. Ruff, Mitlehner, and Helbig [55] first did it for 6H and Lades [40] later followed for 4H-SiC by fitting to the results in Eq. (7) with N the and $N_{\mathrm{n,p}}$.

$$\Delta E_{\mathrm{g}} = C_{\mathrm{n,p}}\left(\ln\left(\frac{N}{N_{\mathrm{n,p}}}\right) + \sqrt{\left(\ln\left(\frac{N}{N_{\mathrm{n,p}}}\right)\right)^{2} + G}\right) \tag{9}$$

A more physically based approach is to interpret the band gap reduction as renormalization due to electron-electron interactions alone. To describe this effect Schubert [50] proposed the band gap narrowing described by Eq. (10).

$$\Delta E_{\mathrm{g}} = \frac{e^{2}}{4\pi\varepsilon r_{\mathrm{s}}} \tag{10}$$

The screening radius r_{s} is given by the Debye and Thomas-Fermi radii leading to the descriptions for the non-degenerate (see Eq. (11)) and generate (see Eq. (12)) case with n the charge carrier concentration.

$$\Delta E_{\mathrm{g}} = \frac{e^{3}\sqrt{n}}{4\pi\varepsilon^{3/2}\sqrt{k_{\mathrm{B}}T}} \quad \text{(Debye, non-degenerate)} \tag{11}$$

$$\Delta E_{\mathrm{g}} = \frac{e^{3}\sqrt{m^{*}_{\mathrm{de}}(3n)^{1/3}}}{4\pi^{5/3}\varepsilon^{3/2}\hbar} \quad \text{(Thomas-Fermi, degenerate)} \tag{12}$$

We want to highlight that in state-of-the-art TCAD tools only Eq. (4) and Eq. (9) are supported out of the box, although some feature the possibility to write custom code for band gap narrowing.

B. Results & Discussion

Multiple methods to determine the band gap, which were partially discussed by De Napoli [56], Nava *et al.* [57], were used in literature. Most of them focus on measurements, e.g., transmission spectroscopy (TS)[34,58], spectroscopic ellipsometry[59], photo absorption (PA)[23,24,46,60], optical admittance (OA)[61], exciton electroabsorption (EE)[20], free carrier absorption (FCA)[38], free exciton luminescence (FEL)[19], photoluminescence (PL)[16,21,62], photoconductivity (PC)[63] and wavelength-modulated absorption (WMA)[22,64]. Sometimes the results of multiple measurements

are combined to improve the accuracy[12]. Stefanakis and Zekentes[65] states that the free carrier absorption method overestimates the band gap while optical absorption studies deliver more accurate results.

An alternative are calculations, which include empirical pseudopotentials (EP)[66–69], density functional theory local density approximation (DFT-LDA)[3,5,30,70–76], rectangular barrier of finite height (RB)[77]. fitting (FT)[27,40,78,79] and genetic algorithm fitting (GAF)[80].

With these methods mainly results for low temperatures were achieved (see Table I). Predominantly the exciton band gap energy was measured, whereat the achieved values seem to agree on $E_{gx} = (3.265 \pm 0.002)\,\mathrm{eV}$. For the band gap energy only two investigations could be found which deliver $E_g = 3.285\,\mathrm{eV}$ respectively $E_g = 3.28\,\mathrm{eV}$. The calculations show a much larger spread, however, the latest investigations all propose significantly lower values of $E_g = (3.15 \pm 0.03)\,\mathrm{eV}$. For room temperature only few dedicated measurements are available[38,46,58,59,81], whereat the ones by Ahuja *et al.*[58] have a quite big uncertainty of 98 meV. We only found one publication that investigated the anisotropy[46] achieving the same exciton (band gap) energy for fields parallel resp. perpendicular to the c-axis. The doping induced band gap narrowing is in general not known for these measurements.

TABLE I: Band gap energies and their temperature dependency fittings. If no temperature dependency parameters (for Eq. (4)) are shown T_g represents the measurement temperature for the shown energies. Highlighted (blue) lines represent no 4H results and (purple) calculations.

ref.	band gap E_g [eV]	E_{gx} [eV]	E_x [meV]	temperature dep. T_g [K]	α [eV K^{-1}]	β [K]	interval [K]	method[82]
[Choy57][60 83]	-	-	-	-	3.3×10^{-4}	-	-	PA
[Choy64][24]	-	3.263 ± 0.003	-	4	-	-	-	PA
[Choy64a][23 84]	-	3.265	-	4.7	-	-	-	PA
[Jung70][68]	2.8	-	-	0	-	-	-	EP
[Dubr75][20]	-	-	20 ± 15	2	-	-	-	EE
[Dubr77][77]	3.2	-	-	0	-	-	-	RB
[Iked80b][19]	-	3.2639	10	77	-	-	-	FEL
[Gavr90][85]	2.89	-	-	0	-	-	-	DFT-LDA
[Back94][66]	3.28	-	-	0	-	-	-	EP
[Park94][86]	2.14	-	-	0	-	-	-	EP
[Kord95][21]	-	3.265	-	4.2	-	-	-	PL
[Wenz95][87]	3.56	-	-	0	-	-	-	DFT-LDA
[Evwa96][61]	3.41 ± 0.03	-	-	40	-	-	-	OA
[Itoh96][16 84]	-	3.265	-	4.25	-	-	-	PL
[Kaec96][88]	2.18	-	-	0	-	-	-	DFT-LDA
[Bako97][89]	3.19	-	-	300	3.3×10^{-4}	0	300–700	FT

[Chen97][70]	3.27	-	-	0	-	-	-	DFT-LDA
[Pers97][73]	2.9	-	-	0	-	-	-	DFT-LDA
[Vanh97][69]	3.28	-	-	0	-	-	-	EP
[Ivan98][62]	-	3.266	-	2	-	-	-	PL
[Bell00][67]	3.05	-	-	0	-	-	-	EP
[Lade00][40][90]	-	3.265	40	0	3.3×10^{-4}	1.05×10^{3}	4–200	FT
	-	3.265	40	0	3.3×10^{-2}	1×10^{5}	4–600	FT
	-	3.342	40	0	3.3×10^{-4}	0	300–700	FT
[Srid00][64]	-	3.267	-	2	-	-	-	WMA
[Zhao00a][76]	3.11	-	-	0	-	-	-	DFT-LDA
[Levi01][79][91]	3.23	-	-	300	6.5×10^{-4}	1300	-	FT
[Ahuj02][58]	3.260 ± 0.098	-	-	300	-	-	-	TS
[Gale02][38]	3.285	-	-	0	3.5×10^{-4}	1100	0–650	FCA
	3.2625	-	-	300	2.4×10^{-4}	0	300–650	FCA
[Ivan02][63]	3.285	-	20.5 ± 1.0	2	-	-	-	PC
[Shal02][81]	3.18	-	-	300	-	-	-	PL
[Dong04][71]	2.194	-	-	0	-	-	-	DFT-LDA
[Son04][5]	3.35	-	-	0	-	-	-	DFT-LDA
[Bala05][43][92]	3.26	-	-	300	4.15×10^{-4}	-131	-	-
[Chin06][3]	2.433	-	-	0	-	-	-	DFT-LDA
[Griv07][46]	-	3.267	30 ± 10	0	-	-	0–500	PA
[Tama08a][93][92]	3.23	-	-	300	7.036×10^{-4}	1509	-	-
[Ng10][80]	3.28	-	-	0	-	-	-	GAF
[Hata13][78][91]	3.285	3.265	20	0	9.06×10^{-4}	2030	0–800	FT
[Kimo14a][27][91]	-	3.265	20	2	8.2×10^{-4}	1800	-	FT
[Yama18][75]	3.12	-	-	0	-	-	-	DFT-LDA
[Kuro19][30]	3.15	-	-	0	-	-	-	DFT-LDA
[Klah20][22]	-	3.2659	40	1.4	-	-	-	WMA
[Lech21][94][92]	3.265	-	-	0	10.988×10^{-3}	32 744.3	-	FT
[Lu21][72]	3.17	-	-	0	-	-	-	DFT-LDA
[Chen22][34]	3.44	-	-	0	5.27×10^{-4}	0	300–620	TS
[Huan22b][95]	3.18	-	-	0	-	-	-	DFT-LDA
[Torr22][74]	3.17	-	-	0	-	-	-	DFT-LDA
[Khan23][96][92]	3.285	-	-	0	3.3×10^{-4}	240	-	-
[Main24][59]	3.30 ± 0.02	-	-	300	-	-	-	SE

The free exciton binding energy E_x was first estimated by Hagen, Van Kemenade, and Van Der Does De Bye[97] to be around 20 meV, with the side note that further investigations are needed. Later, five measurements were published[19,20,22,46,63]. The achieved values range from 10–40 meV. The value of 10 meV[19] was determined for the activation energy for thermal quenching of free excitons, however, Devaty and Choyke[98] argue that these values are too low to be free exciton binding energies.

1. *Temperature Dependency*

Very few measurements on the temperature dependency are available[23,34,38,46]. The remaining models[27,40,78,79] fit the data published by Choyke [12], Choyke, Patrick, and Hamilton [23], Choyke, Hamilton, and Patrick [24] from the 1960s. Surprisingly, the model development only started at the beginning of the 2000s. In 1997 Bakowski, Gustafsson, and Lindefelt [89] were still forced to use the 6H values. In 2004 Ayalew [99] stated that not reliable data are available.

The origin of some of the proposed model parameters[43,94,96] could not be traced back to any scientific publication. Occasionally, we were able to them back to prominent TCAD simulation suites, where these were used as default values. Although Tamaki *et al.* [93] provides a reference for the used model[100], we were unable to verify the parameters. By comparison we found that the results are very close to those predicted by Kimoto and Cooper [27] (see Fig. 1).

To describe the temperature dependency the majority resorts to the Varshni model (see Eq. (4)). We would like to highlight that the value $\alpha = 3.3\times10^{-4}\,\mathrm{eV\,K^{-1}}$ was determined by Choyke and Patrick [60] for an undefined polytype of SiC. According to the utilized band gap we suspect it to be 21R-SiC device although Bakowski, Gustafsson, and Lindefelt [89] argued that it was 6H. Nevertheless, a wide range of fittings utilizes this value, i.e., that 4H and 6H share the same temperature dependency[101]. Nallet *et al.* [102] even references 6H values directly[55], which, however, go back to the same data by Choyke and Patrick [60].

The model presented in Eq. (6) is solely used by Grivickas *et al.* [46] with the parameters shown in Eq. (13).

$$\Theta_\mathrm{p} = 450\,\mathrm{K}, \qquad \varepsilon = 3\times10^{-4}\,\mathrm{eV\,K^{-1}}, \qquad p = 2.9\,. \tag{13}$$

From a graphical representation of the band gap energy versus temperature (see Fig. 1) the deviations of the models becomes evident. We do not show the fitting by Hatakeyama, Fukuda, and Okumura [78] which is identical to the one by Kimoto and Cooper [27]. Similarly, the parameters provided by Lechner [94] reproduce the fitting from Lades [40] (4–600 K).

First of all it has to be noted that the measurements nicely distinguish E_g and E_gx. The same can not be said for the fittings. For example, Levinshteĭn, Rumyantsev, and Shur [79] denoted to describe E_g but the values agree more to E_gx. Also the fitting by Bakowski, Gustafsson, and Lindefelt [89], who simply took the band gap at 0 K and applied the scaling factor α, turns out to underestimate the band gap. Newer models, e.g., the one by Cheng, Yang, and Zheng [34], suggest a much different slope with temperature, actually crossing the traces of E_gx with E_g. The model by

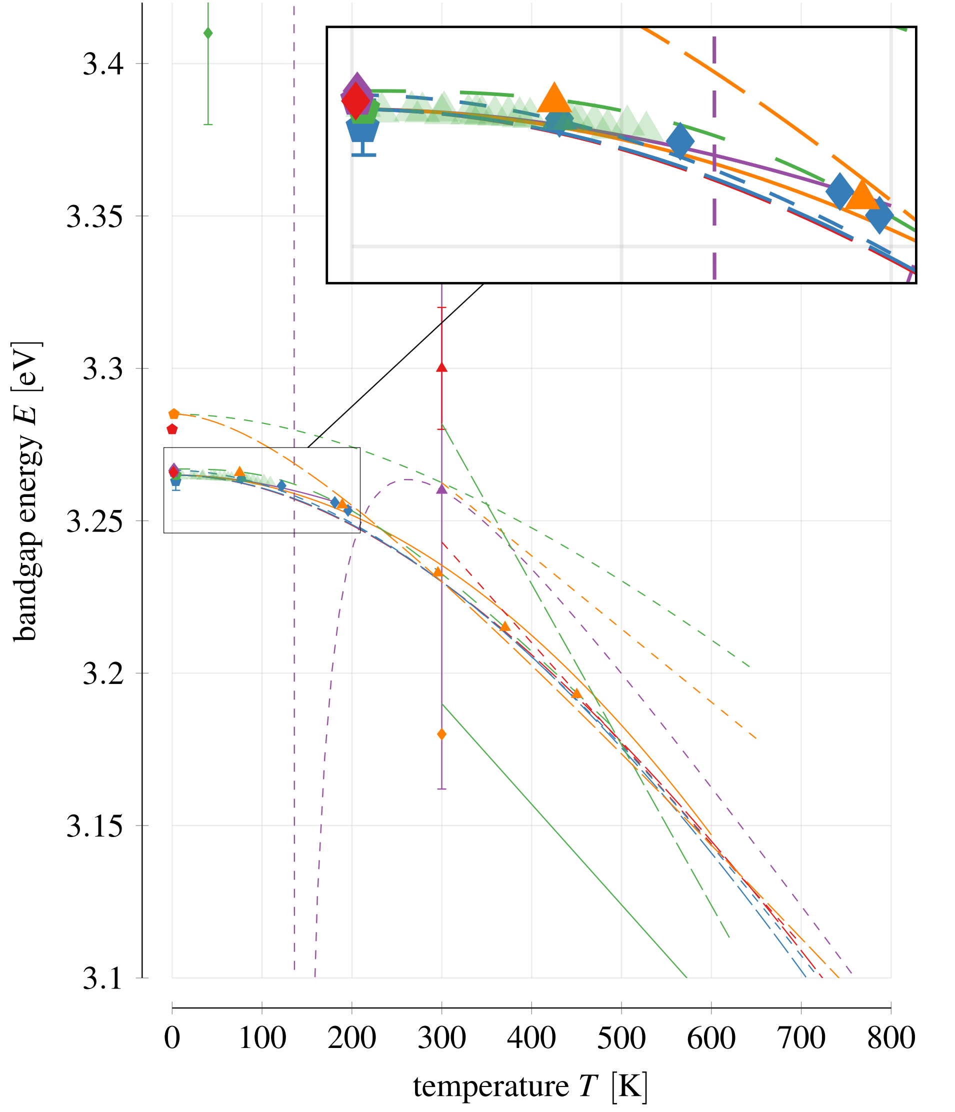


FIG. 1. Band gap measurements and models. The latter are, if available, only shown in the specified confidence interval. (V) denotes a fitting using the Varshni model and (P) fitting with the Pässler model.

TABLE II. Parameters for ionized dopants induced band gap narrowing.

ref.	method	n-type A_{nc} [meV]	B_{nc} [meV]	A_{nv} [meV]	B_{nv} [meV]	p-type A_{pc} [meV]	B_{pc} [meV]	A_{pv} [meV]	B_{pv} [meV]	C_{pv} [meV]
[Lind98][52]	calculation	-15	-2.93	19	8.74	-15.70	-0.39	13	1.15	-
[Pers99][53]	calculation	-17.91	-2.20	28.23	6.24	-16.15	-1.07	-35.07	6.74	56.96

Khanna [96] matches E_g at low temperatures but at around 200 K it is equal to E_{gx} and follows that value from there onward. The fitting by Balachandran, Chow, and Agarwal [43] is only feasible for $T \geq 300$ K as it has a singularity at 131 K.

The plateau achieved by the Pässler model in Eq. (6) is barely visible, showing that the deviations are only subtle. Lades [40] approximated the shape with the Varshni model by just fitting it in a very narrow temperature range. The phonon dispersion of 4H-SiC $\Delta = 0.29$[46] is rather low, which would actually indicates that Eq. (5) is the most suitable, however, Eq. (6) seems to be accurate as well. Even more, Stefanakis and Zekentes [65] compared the single models and identifies Eq. (4) as the most suitable one. In fact, we did not find a single instance where Eq. (5) was used to describe 4H-SiC.

2. *Doping Dependency*

Two fittings for the doping dependent narrowing model in Eq. (7) could be found (see Table II). We want to highlight that these are solely based on calculations. Measurement results are available[46,103], but due to their sparsity (see Fig. 3) they are not suitable to verify the calculations.

The main issue we identified regarding the parameters is an incorrect sign, as often all parameters become negative (see Fig. 2). The fact that in some cases, e.g., by Lophitis *et al.* [104], the Jain-Roulston form is used (see Eq. (8)) makes a direct comparison of the parameters challenging. Furthermore, the parameter for the term with exponent $1/2$ are sometimes combined[11,105,106], which makes it potentially impossible to apply them accurately in certain TCAD tools. A detailed analysis of all the inconsistencies we found in literature is provided in **??**.

For the Slotboom model, that is used by various publications[40,94,99], one set of parameters is available[40] (see Table III). In contrast to the other models the band gap narrowing is linear in the

Lindefelt $(A_{\mathrm{nc}}, A_{\mathrm{nv}})$ $(B_{\mathrm{nc}}, B_{\mathrm{nv}})$ $(A_{\mathrm{pc}}, A_{\mathrm{pv}})$ $(B_{\mathrm{pc}}, B_{\mathrm{pv}})$ (C_{pv})

Lindefelt

- [Lind98][52] $(-1.5\times10^{-2}, 1.9\times10^{-2})$ $(-2.93\times10^{-3}, 8.74\times10^{-3})$ $(-1.57\times10^{-2}, 1.3\times10^{-2})$ $(-3.87\times10^{-4}, 1.15\times10^{-3})$ (-)
  - [Levi01][79] $(-1.5\times10^{-2}, 1.9\times10^{-2})$ $(-2.93\times10^{-3}, 8.74\times10^{-3})$ $(-1.57\times10^{-2}, 1.3\times10^{-2})$ $(-3.87\times10^{-4}, 1.15\times10^{-3})$ (-)
  - [Well01][107] (- , -) (- , -) (- , -) (- , -) (-)
  - [Cha08][108] $(-1.5\times10^{-2}, 1.9\times10^{-2})$ $(-2.93\times10^{-3}, 8.74\times10^{-3})$ (- , -) (- , -) (-)
    - [Chen12][109] $(-1.5\times10^{-2}, 1.9\times10^{-2})$ $(-2.93\times10^{-3}, 8.74\times10^{-3})$ (- , -) (- , -) (-)
  - [Alba10][11] $(-1.5\times10^{-2}, 1.9\times10^{-2})$ (1.7×10^{-2}) $(1.57\times10^{-2}, 1.3\times10^{-2})$ (1.54×10^{-2}) (-)
  - [Zhan10][110] $(-1.5\times10^{-2}, 1.9\times10^{-2})$ $(-2.93\times10^{-3}, 8.74\times10^{-3})$ (- , -) (- , -) (-)
  - [Bell11][105] $(-1.5\times10^{-2}, 1.9\times10^{-2})$ (1.17×10^{-2}) $(1.57\times10^{-2}, 1.3\times10^{-2})$ (1.54×10^{-3}) (-)
  - [Habi11][31] $(-1.5\times10^{-2}, 1.9\times10^{-2})$ $(-2.93\times10^{-3}, 8.74\times10^{-3})$ $(-1.57\times10^{-2}, 1.3\times10^{-2})$ $(-3.87\times10^{-4}, 1.15\times10^{-3})$ (-)
  - [Buon12][111] $(-1.5\times10^{-2}, -1.9\times10^{-2})$ $(-2.93\times10^{-3}, -8.74\times10^{-3})$ (- , -) (- , -) (-)
  - [Pezz13][106] $(1.5\times10^{-2}, 1.9\times10^{-2})$ (1.17×10^{-2}) $(1.57\times10^{-2}, 1.3\times10^{-2})$ (1.54×10^{-3}) (-)
  - [Stef14][65] $(-1.5\times10^{-2}, 1.9\times10^{-2})$ $(-2.93\times10^{-3}, 8.74\times10^{-3})$ $(-1.57\times10^{-2}, 1.3\times10^{-2})$ $(-3.87\times10^{-4}, 1.15\times10^{-3})$ (-)
  - [Zegh19][112] $(-1.5\times10^{-2}, 1.9\times10^{-2})$ (1.17×10^{-2}) $(-1.37\times10^{-2}, 1.3\times10^{-2})$ (1.54×10^{-3}) (-)
  - [Zegh20][113] $(-1.5\times10^{-2}, 1.9\times10^{-2})$ (1.17×10^{-2}) $(-1.37\times10^{-2}, 1.3\times10^{-2})$ (1.54×10^{-3}) (-)
  - [Ioff23][4] $(-1.5\times10^{-2}, -1.9\times10^{-2})$ $(-2.93\times10^{-3}, -8.74\times10^{-3})$ $(-1.57\times10^{-2}, -1.3\times10^{-2})$ $(-3.87\times10^{-4}, -1.15\times10^{-3})$ (-)
  - [Maxi23][114] $(-1.5\times10^{-2}, -1.9\times10^{-2})$ $(-2.93\times10^{-3}, -8.74\times10^{-3})$ $(-1.57\times10^{-2}, -1.3\times10^{-2})$ $(-3.87\times10^{-4}, -1.15\times10^{-3})$ (-)

Persson, Lindefelt, and Sernelius

- [Pers99][53] $(-1.791\times10^{-2}, 2.823\times10^{-2})$ $(-2.2\times10^{-3}, 6.24\times10^{-3})$ $(-1.615\times10^{-2}, -3.507\times10^{-2})$ $(-1.07\times10^{-3}, 6.74\times10^{-3})$ (5.696×10^{-2})
  - [Nipo16][115] (- , -) (- , -) (- , -) (- , -) (-)
  - [Loph18][104] $(-1.791\times10^{-2}, 2.823\times10^{-2})$ $(-2.2\times10^{-3}, 6.24\times10^{-3})$ $(-7.311\times10^{-2}, 3.507\times10^{-2})$ $(-1.07\times10^{-3}, 6.74\times10^{-3})$ (-)

Slotboom $(C_{\mathrm{n}}, N_{\mathrm{n}} \mid C_{\mathrm{p}}, N_{\mathrm{p}} \mid G)$

Lades

- [Lade00][40] $(2\times10^{-2}, 1\times10^{17} \mid 9\times10^{-3}, 1\times10^{17} \mid 5\times10^{-1})$
  - [Ayal04][99] $(2\times10^{-2}, 1\times10^{17} \mid 9\times10^{-3}, 1\times10^{17} \mid 5\times10^{-1})$
  - [Lech21][94] $(2\times10^{-2}, 1\times10^{17} \mid$ - , - $\mid 5\times10^{-1})$

FIG. 2. Citations and extracted parameters for the doping dependency of the band gap. If solely a single value is shown for parameter B then the publication only provides $B_{\mathrm{c}}+B_{\mathrm{v}}$. [green box] are fundamental investigations and [orange box] connections predicted from the used values.

semi-logarithmic plot (see Fig. 3). In a reasonable doping concentration range the deviation for p-type material is quite low but for n-type material considerable. The models of[52] and[53] only differ by a small amount.

The band gap narrowing according to Eq. (12) is also shown, because is it also occasionally used[54,65], whereat Stefanakis and Zekentes [65] used a slightly different form of the Thomas-Fermi radius shown in Eq. (14) with n_0 the equilibrium carrier density.

$$\Delta E_{\mathrm{g}} = \frac{e^2}{4\pi\varepsilon_0\varepsilon_{\mathrm{s}}}\left(\frac{3n_0e^2}{2\varepsilon_0 E_{\mathrm{F}}}\right)^{1/2} \tag{14}$$

Unfortunately our calculations did not succeed to reproduce the results achieved in these publica-

TABLE III. Parameters for ionized dopants induced band gap narrowing Slotboom model.

ref.	type	C [eV]	N [cm^{-3}]	G [1]
[Lade00][40]	n	2×10^{-2}	10^{17}	0.5
	p	9×10^{-3}	10^{17}	0.5

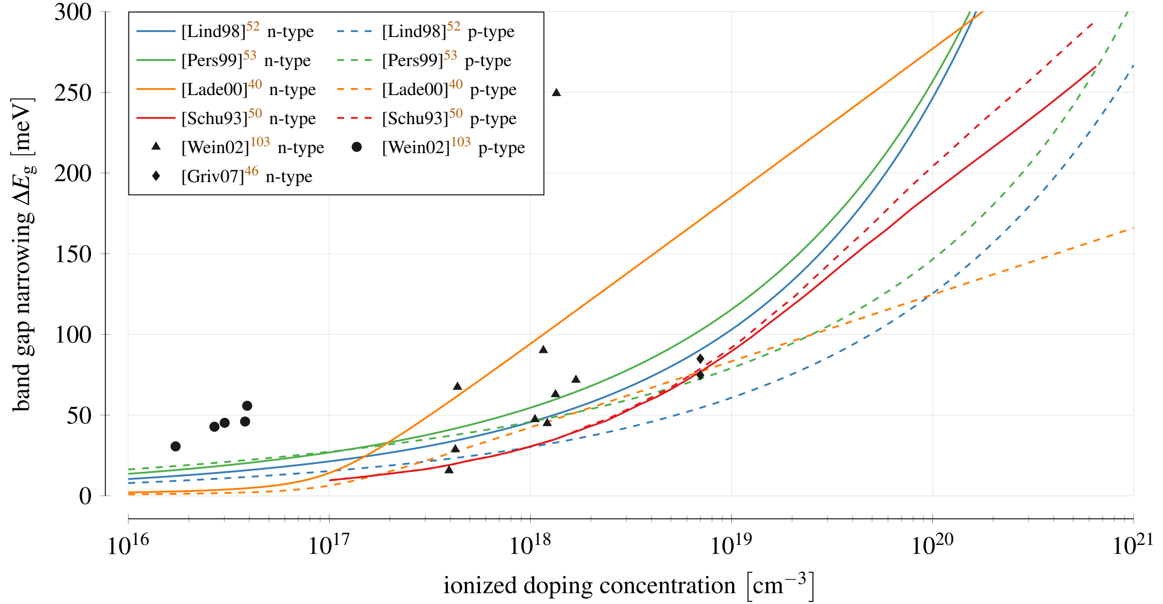


FIG. 3. Doping induced band gap narrowing. The different models complemented by measurement results for p- and n-type material are shown.

tions so we extracted the curve from Donnarumma, Palankovski, and Selberherr [54]. Surprising for us is also the shape of the narrowing, which becomes almost linear in the semi-logarithmic plot for high doping concentrations. With the simple assumption $n = N_D^+$ resp. $n = N_A^-$ this does not seem to be possible. Last Johannesson and Nawaz [116] used the Debye radius from Eq. (11), based on the calculations by Lanyon and Tuft [117].

3. *TCAD Values*

An overwhelming amount of band gap values can be found in literature (see Fig. 4). Measurements mainly focused on the exciton band gap energy E_{gx} at low temperatures, resulting in values

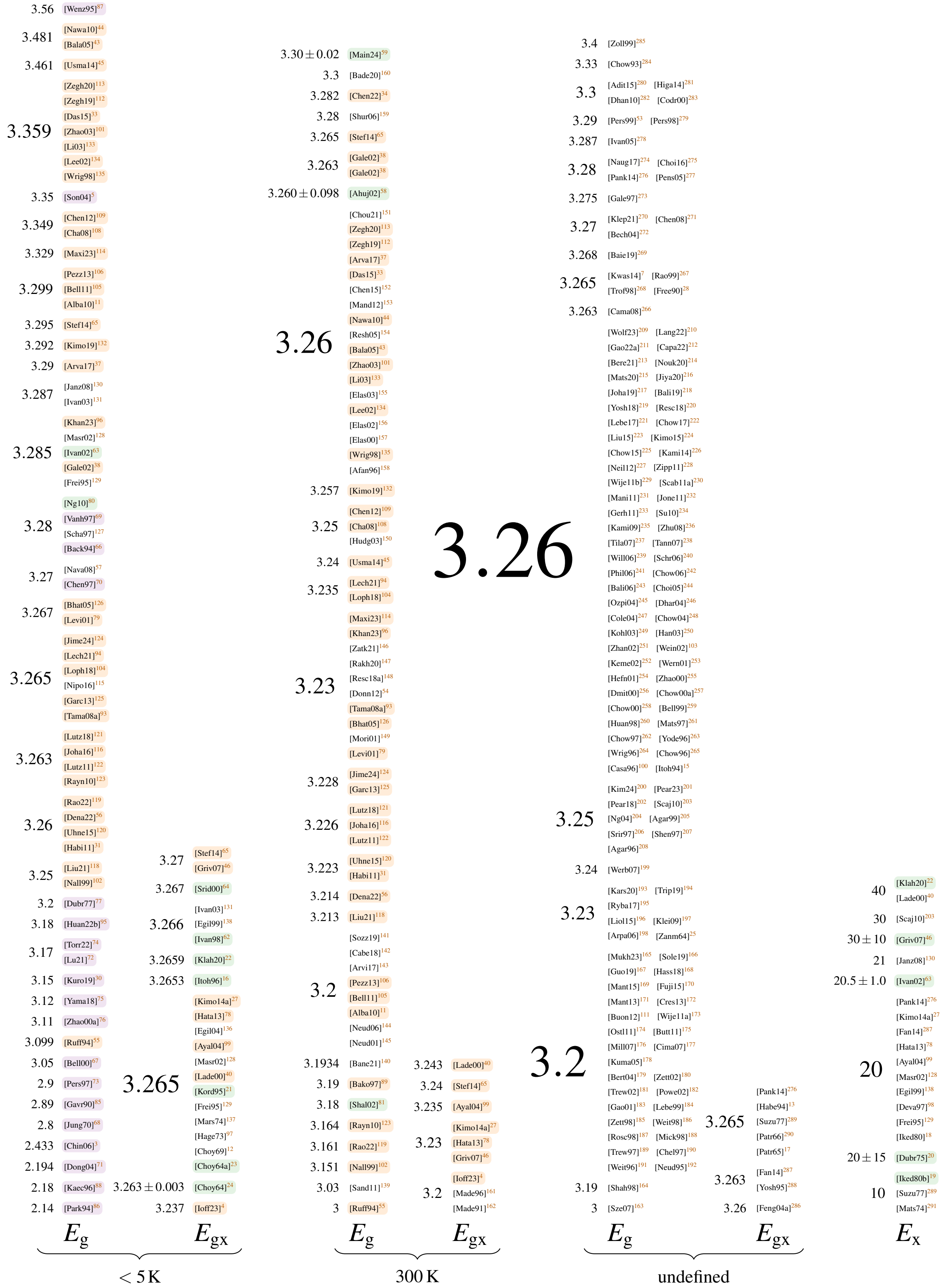


FIG. 4. Values for band gaps at varying temperatures. ▪ values correspond to calculations, ▪ ones to measurements and ▪ ones are values calculated from models.

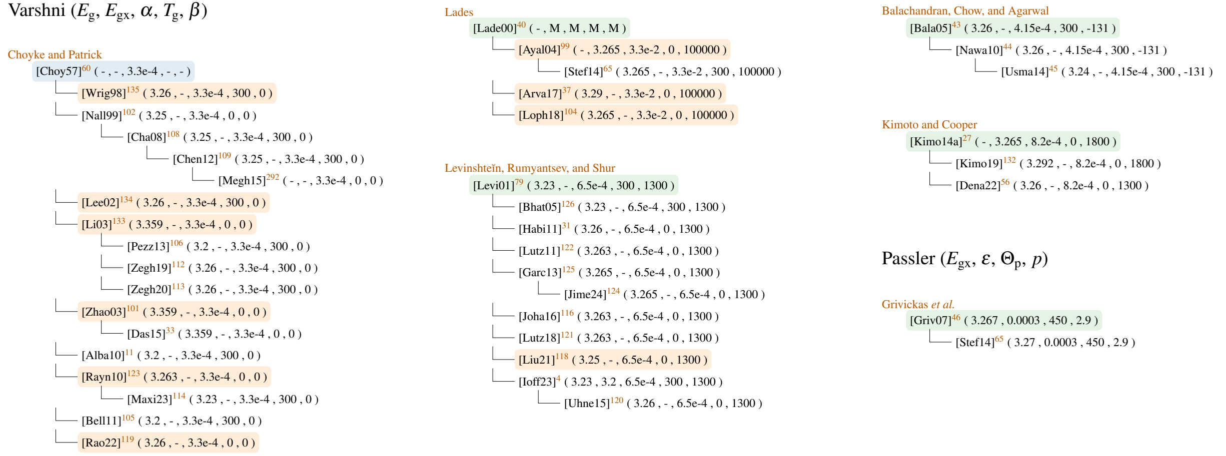


FIG. 5. Citations and the respective values for the temperature dependency. entries indicate values that have not been determined for 4H-SiC, are fundamental investigations and connections predicted from the used values.

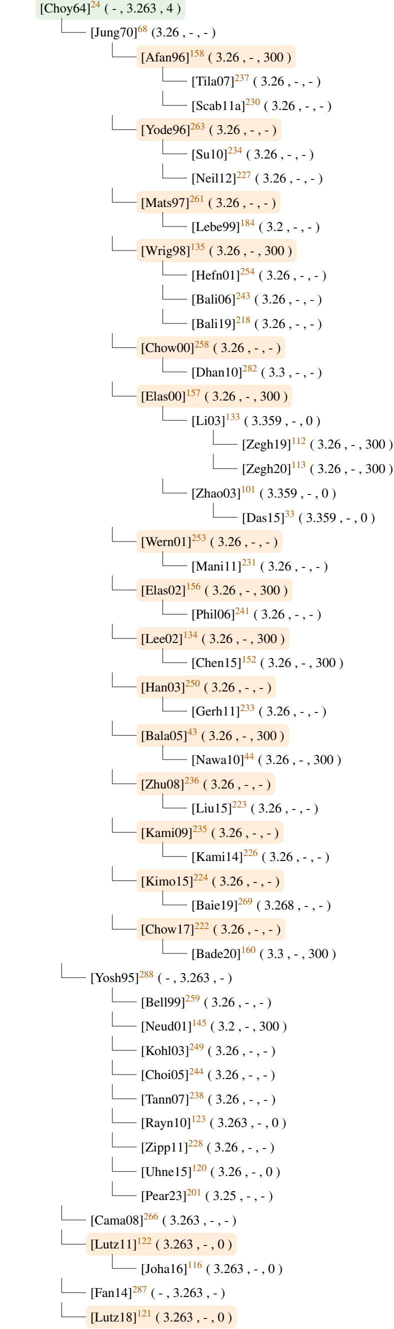
of (3.265 ± 0.002) eV. Using the broadly accepted value of $E_x = 20$ meV (see also Fig. 7) a band gap energy of $E_g = 3.285$ eV is achieved, which has also been confirmed by dedicated measurements. The additional higher and lower values mainly stem from temperature dependency models, which were designed for higher temperatures and, thus, lack accuracy at low one. In general, only a few values for the parameters α and β are used (see Fig. 5), however, the energy value ($E_g(T_g)$ in Eq. (3)) is varied resulting in this wide range of values. Also calculations often deviate significantly. At room temperature few measurements are available such that values are dominated by model fitting.

The question that remains to be answered is on which values the various models for the band gap E_g are based upon, since there are very few measurements available. Our analysis revealed that it sound to assume, that all the values currently in use go back to the investigations of E_{gx} by Choyke, Patrick, and Hamilton [23], Choyke, Hamilton, and Patrick [24] in 1964. Already in 1970 Junginger and Van Haeringen [68] rounded the achieved values of $E_{gx} = 3.263$ eV to $E_g = 3.26$ eV. The same things were observed for the results from Choyke, Patrick, and Hamilton [23], i.e., $E_{gx} = 3.263$ eV. Stunningly, not only the value was changed but the exciton band gap energy was turned into the band gap energy, completely neglecting the free exciton binding energy. In fact, the excitonic values are nowadays only encountered in sophisticated publications.

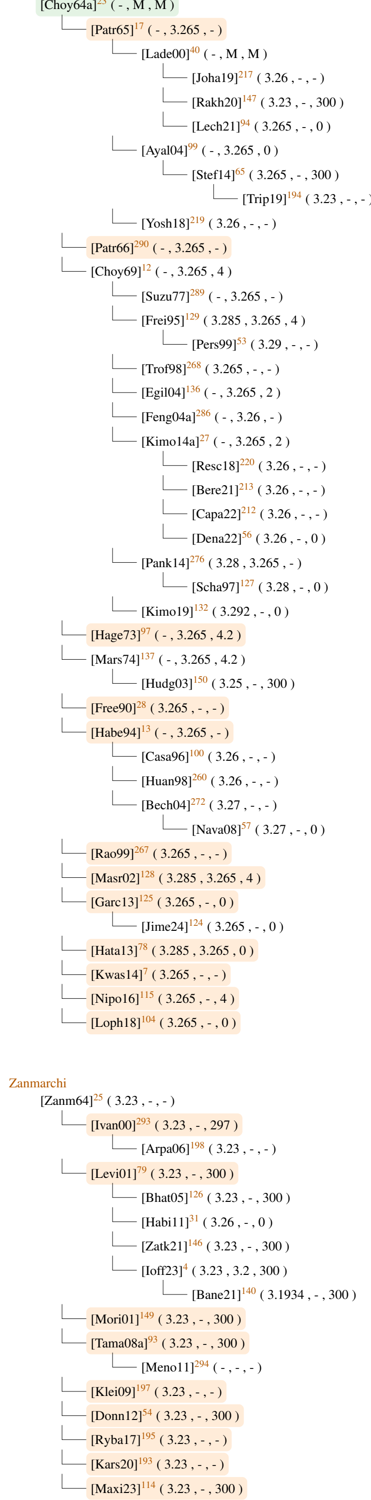
Zanmarchi [25] introduced in 1964 for the first time the value $E_g = 3.23$ eV, which is also commonly used today. Due to missing data at that time it is reasonable to assume that it was derived

Band Gap (E_g, E_{gx}, T)

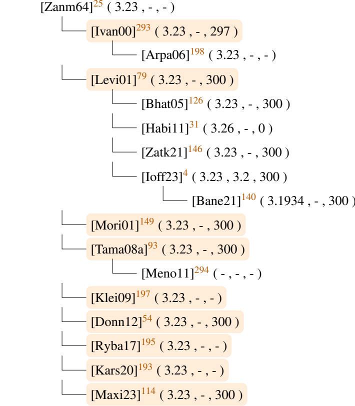
Choyke, Hamilton, and Patrick



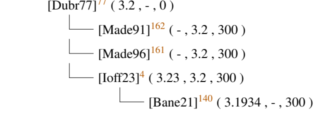
Choyke, Patrick, and Hamilton



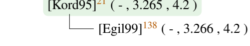
Zanmarchi



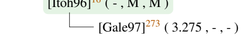
Dubrovskii and Lepneva



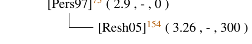
Kordina *et al.*



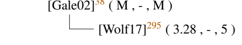
Itoh, Tsunenobu Kimoto, and Hiroyuki Matsunami



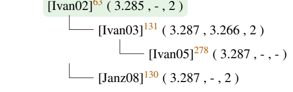
Persson and Lindefelt



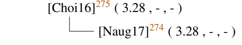
Galeckas *et al.*



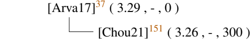
Ivanov *et al.*



Choi



Arvanitopoulos *et al.*



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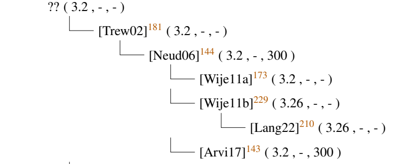

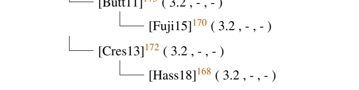

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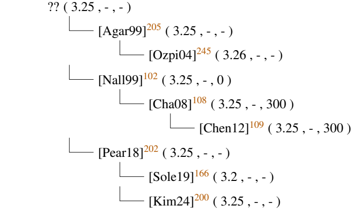

FIG. 6. Citations and values for band gap energies. ▇ are fundamental investigations and ▇ connections predicted from the used values. We collect publications that share the same value but that do not provide a reference under ??.

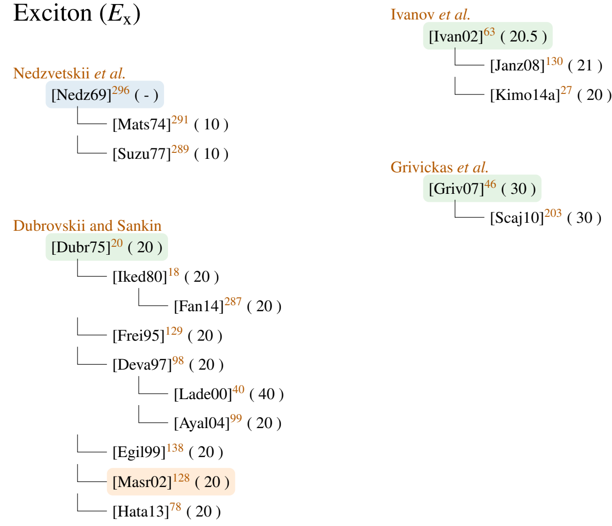

FIG. 7. Citations and values of the free exciton binding energy E_x. entries indicate values that have not been determined for 4H-SiC, are fundamental investigations and connections predicted from the used values.

based on low temperature measurements of the exciton band gap. Also $E_g = 3.2\,\text{eV}$ seems to result from rounding $E_g = 3.265\,\text{eV}$. This was values was also achieved by Dubrovskii and Lepneva [77] who added the exction band gap $E_{gx} = 3.265\,\text{eV}$[12] and $E_x = 20\,\text{meV}$ to achieve $E_g = 3.2\,\text{eV}$. Solely for $E_g = 3.25\,\text{eV}$ we have no clear explanation, but maybe it is simply the result of a typographical error when transferring $E_g = 3.265\,\text{eV}$.

The outcome of our analysis is thus, that it is possible that the room temperature band gap energies commonly used in literature go back to low temperature exciton band gap energy measurements six decades ago. The fact that Ahuja *et al.* [58] achieved the same value of $E_g = 3.23\,\text{eV}$ as Zanmarchi [25] 60 years ago shows, that multiple avenues to a specific values are possible and thus such statements not easy to prove. Nevertheless, since we did not find any other derivations, we think that the chances that our hypothesis is true is quite high.

Aren't that horrifying news? Well, coincidentally recent measurements by Galeckas *et al.* [38] and Ahuja *et al.* [58] actually suggest that the band gap energy at 300 K is approximately 3.26 eV, whereat it has to be noted that the result by the latter have an uncertainty of 98 meV and thus have to be handled with care. To confirm that $E_{gx}(0) \approx E_g(300)$ holds, additional verifications are required. In our opinion this also includes an investigation of E_x versus temperature, which is assumed constant at the moment. The newest models (see Fig. 1), however, suggest an increasing distance between the band gap energies.

An additional avenue for future research would be an investigation of the differences between measurements and calculations. If the latter achieve the actually more accurate results the band gap energy for 4H-SiC might need significant corrections.

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