

Electroluminescence Spectra of a Gate Switched MOSFET at Cryogenic and Room Temperatures Agree with Ab Initio Calculations of 4H-SiC/SiO₂-Interface Defects

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Abstract. To reach the theoretical performance limit of 4H-SiC MOSFETs the SiC/SiO₂-interface defects along the inversion channel need to be fully identified. We employ a measurement technique that allows to observe energetically resolved trap states at the SiC/SiO₂-interface by measuring the electroluminescence of a gate pulsed MOSFET. The spectra are recorded at room and cryogenic temperatures with a spectrometer and two different amplitudes of the gate pulse. Comparison of the results to literature allows for identification of the L₁ line of the D₁ center with an energy of 2.9 eV and suggests donor-acceptor-pair recombination or Z_{1/2} to be responsible for the emission around 2.5 eV. Ionization energies of P_{bc} and related vacancy centers determined via ab initio calculations show similar results as the experimental data and provide a possible classification of the trap level around 1.8 eV.

Introduction

Silicon carbide (SiC) with its superior material properties is well suited for high power metal-oxide-semiconductor field-effect transistors (MOSFETs). However, the inversion channel field-effect mobilities are still below the theoretical expectations [1]. Charge carriers flowing through the channel of a MOSFET can get trapped at SiC/SiO₂-interface states affecting the device performance. The density of trapped carriers at the interface can be obtained by e.g. measuring the subthreshold sweep hysteresis in the drain current when switching the MOSFET between on- and off-state [2]. However, the defect structure at an atomic level still remains an open question despite numerous previous studies. When the atomic defect configurations of interface traps are known, the development of defect density reducing techniques is facilitated. Here, we use energy-resolved electroluminescence measurements [3, 4, 5, 6] at cryogenic temperatures in combination with ab initio calculations to characterize the SiC/SiO₂-interface. During the measurement the gate is switched between accumulation and inversion which results in radiative carrier recombinations via mid gap defects. The focus of the theoretical approach lies on carbon dangling bonds (P_{bc}) as they have been found in similar devices with electrically detected magnetic resonance (EDMR) [7], a measurement approach which is as well sensitive to mid gap states.

Electroluminescence at the 4H-SiC/SiO₂-Interface of a MOSFET

The experimental part to characterize SiC/SiO₂-interface states is based on the spectroscopic detection of photons released by radiative recombination of trapped charges with charge carriers from the valence or conduction band. We continuously pulse a 4H-SiC MOSFET test structure via the gate terminal between accumulation and inversion resulting in a periodic recombination of electrons and

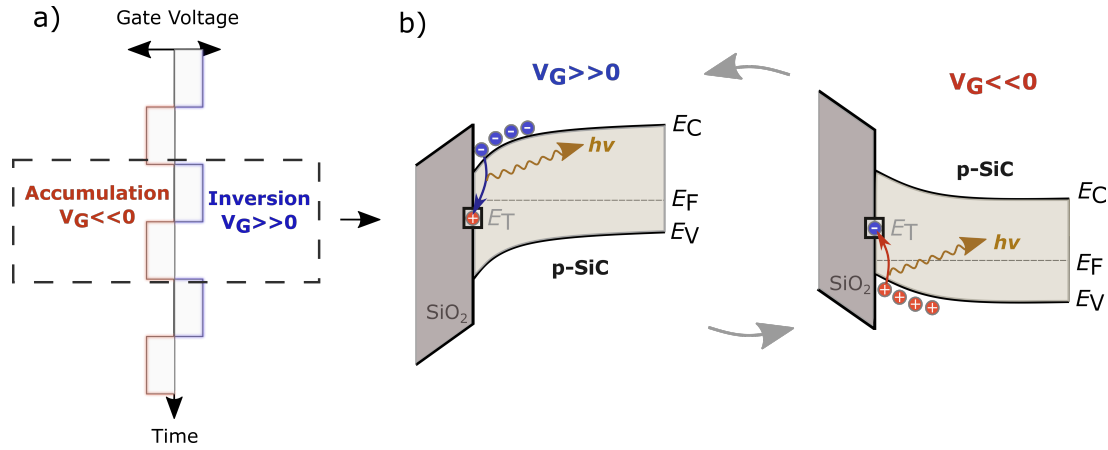


Fig. 1: (a) Repeated pulsing of the gate between accumulation and inversion with a frequency of 1.5 MHz. (b) Carriers get trapped at interface states in each phase and recombine with incoming carriers during the opposite phase. If it is a radiative recombination process photons are emitted with an energy that is in relation to the trap level.

holes with trapped carriers at interface states as illustrated in Fig. 1. During inversion electrons are present at the interface and can recombine with holes that have been trapped during the previous accumulation pulse. In case a radiative recombination event occurs, the thereby released photon has a specific wavelength and energy. Equivalently during accumulation, previously trapped electrons can recombine with holes from the valence band. The relation between the energy of the emitted photon and the trap level of the involved defect is illustrated in Fig. 2 in a configuration coordinate diagram of the adiabatic potential energy surfaces. During the inversion pulse (Fig. 2(a)) an electron from the conduction band can be for instance thermally trapped by a defect state to minimize its energy. Once the MOSFET is switched into accumulation, there are two branches for the trapped electron to be released again: via a vertical radiative recombination with a hole from the valence band or via a non-radiative multiphonon (NMP) process. After the vertical radiative recombination, there is thermal relaxation of the defect down to the minimum of the potential energy surface. The considerable Franck-Condon-shift causes increased thermal broadening of the emitted photon energy. Fig. 2(b) analogously depicts the trapping dynamics when switching from accumulation to inversion. The captured holes can recombine with electrons from the conduction band emitting photons followed by thermal relaxation. Note that only radiative processes are recorded in electroluminescence measurements.

Experimental Approach

Aside from room temperature measurements, which have been already investigated in [4, 5], we also conducted experiments at cryogenic temperatures to investigate the impact of reduced thermal energy onto the radiative process and to ease defect identification. Once a charge carrier is trapped in a defect state, the branching ratio of radiative versus non-radiative detrapping increases. Hence, the 4H-SiC MOSFET test structure is placed inside a Janis Research CCS-XG/204 refrigerator system under high vacuum of 10^{-5} mBar, where it is glued onto a small sapphire (Al₂O₃) plate (Fig. 3). Gate and source of the MOSFET are connected to a Keithley 3390 arbitrary waveform generator. During the measurement the source is grounded and the gate is pulsed between accumulation and inversion with a frequency of 1.5 MHz. Since the metal drain contact of the MOSFET test structure was removed prior to the experiment, photons generated at the interface by gate pulsing can travel through the SiC bulk and exit the device on the backside as shown in Fig. 3. Due to the wide band gap of SiC (3.26 eV) the absorption of photons in the SiC bulk is considered negligible in the region below 3.26 eV. An additional measurement on doped 4H-SiC samples supported this assumption as no relevant absorption in the presented region of 1.2 eV to 3 eV was detected. The emitted light passes through a SiO₂

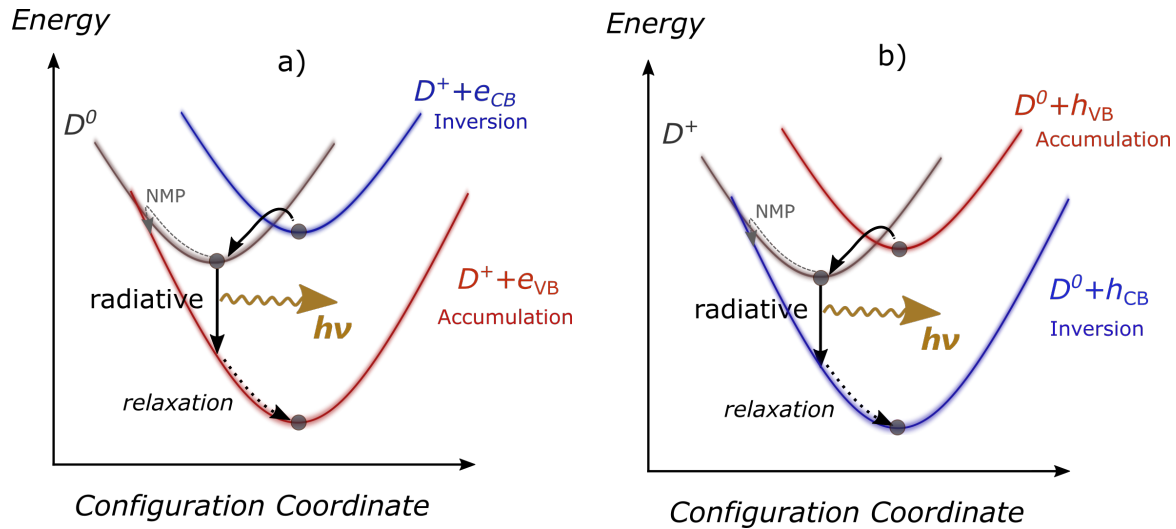


Fig. 2: (a) Configuration diagram representing the trapping dynamics at the example of a positively charged defect D^+ for a gate pulse from inversion to accumulation. Electrons from the conduction band can get trapped in a defect state. Afterwards they can either recombine via a NMP process or recombine with a valence band hole emitting a photon. Radiative recombination with deep traps often is a vertical process that is followed by a relaxation of the defect state via phonons. (b) The equivalent process for a pulse from accumulation to inversion is shown for a trapped hole that can recombine via NMP or radiatively with an electron from the conduction band. (adapted from [4])

window and is then collected by a light guide coupler placed outside the cryostat and connected to an Avantes ULS2048CL spectrometer. The system is shaded from ambient light. Since the minimum integration time of the spectrometer needs to be in the range of seconds, there is no possibility to distinguish between the light emitted during accumulation or inversion. The recorded spectrum is thus the superposition of all radiative emission processes.

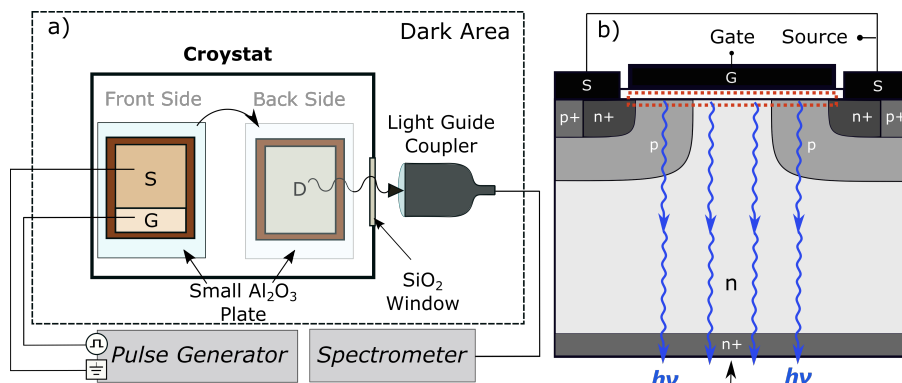


Fig. 3: (a) MOSFET test structure with removed drain contact inside a cryogenic probe station. Source and gate are electrically connected to the pulse generator. The emitted light exits the cryostat via a SiO₂ window, where it is gathered by the light guide coupler. (b) Schematic cross section of the measured MOSFET test structure, where the light is generated at the interface and travels through the SiC bulk and can exit the device due to the removed drain contact.

Theoretical Approach to Model Interface Defects

Defects at the SiC side of the 4H-SiC/SiO₂-interface were modeled based on the abrupt interface model [8] generated following the schemes described in [7]. P_{bC} centers, near interface silicon vacancies ($V_{Si,1}$), and a near interface carbon antisite-vacancy complex ($C_{Si}V_{C,1}$) were considered in our

modelling. P_{bc} centers explain near interfaces defects measured with EDMR as mentioned earlier [7]. The carbon antisite-vacancy complex results from a metastability of $V_{Si,I}$ by an internal transformation as it also occurs in the case of the bulk defects [9]. The interface system was described in the framework of density functional theory (DFT) together with the hybrid exchange-correlation functional HSE06 and the PAW-approach as implemented in the VASP package. Electronic states were represented using an energy cut-off of 420 eV and a k-point sampling using the Γ -point only. The interface with and without defects was represented in an orthorhombic unit cell $15.37 \text{ \AA} \times 15.98 \text{ \AA} \times 28 \text{ \AA}$ with one layer of SiO_2 simulating a thin oxide layer with hydrogen-passivated dangling bonds. Defect ionization levels and the SiC band gap obtained with the hybrid DFT are known to reproduce experimental values well. They represent the direct recombination energies of free holes or electrons (when related to the conduction band edge) with defect levels and were calculated from total energies using standard procedures. Excited states of the defects were obtained using our embedded many-electron approach (CI-CRPA) [10]. This allows to assess the bound exciton recombination. The theoretical lineshape of the direct free-to-bound and bound-exciton recombination was modelled including Franck-Condon shifts and Huang-Rhys factors in the low-temperature high-coupling limit [11].

Experimental Results Compared to Literature

The electroluminescence spectra of the pulsed MOSFET test structure are recorded at cryogenic and room temperatures for two different pulse voltage pairs $\pm 5 \text{ V}$ and $\pm 30 \text{ V}$ (Fig. 4, top). Since the thermal energy is minimized at cryogenic temperature, charges are only provided by field effect ionization. Hence, the amplitude of the voltage pulse is increased from $\pm 5 \text{ V}$ to $\pm 30 \text{ V}$, which increases the probability to charge trap states inside the bandgap especially at low temperatures. The gate pulse of $\pm 30 \text{ V}$ in contrast to the $\pm 5 \text{ V}$ pulsing causes increased electroluminescence especially in the range from 1.6 eV to 2.2 eV at cryogenic temperatures. We can differentiate between electroluminescence coming from the SiC bulk or the SiC/ SiO_2 -interface, by measuring a different SiC diode biased in forward direction. The peak around 2.5 eV appears to originate from SiC bulk states as it appears in both devices (diode and MOSFET). This peak is also reported in literature where the electroluminescence of a forward biased body diode of SiC MOSFETs or the thermal stimulated luminescence in SiC are measured [16, 17, 18, 19, 20, 21, 22]. Tab. 1 summarizes the energetic position and origin of these and other reported peaks in literature. It has been attributed to donor-acceptor-pair recombinations (DAP) involving the defect level termed i-center as acceptor level and nitrogen (N) as donor level [23]. Others, however, suggest this emission from a recombination process via the defect level $Z_{1/2}$ [20, 24]. $Z_{1/2}$ is a well-known electron trap in 4H-SiC with a level at $E_C - 0.63 \text{ eV}$ that fits the experimental data [24]. It is most likely related to the negative carbon vacancy [25]. In accordance with literature this peak is very broad and most pronounced at low temperatures [16, 21], as the probability for the recombination with deeper levels decrease with temperature [26]. The two very sharp peaks around 2.8 eV might stem from oxygen related emissions [27] or from an intrinsic SiO_2 defect level [1]. The very sharp peak at 2.9 eV only appears at cryogenic temperatures especially below 20 K. It has been attributed to the L_1 line of the D_1 center previously [12, 13, 14, 15, 16]. The microscopic defect structure of the D_1 is still under debate. Suggestions range from implantation related defects to intrinsic defect in 4H-SiC. For instance, Storasta *et al.* assume a pseudodonor character of the the D_1 defect, that is associated with a hole trap at 0.34 eV above the valence band [28]. We attribute the electroluminescence between 1.5 eV and 2.2 eV to the interface since it does not appear in any electroluminescence spectrum of the forward biased SiC diodes of our measurement nor in bulk-SiC related literature. As depicted below in the measured spectrum and mentioned in the theoretical section, P_{bc} centers at the interface [7] could explain the electroluminescence in this energy range. The rough interface between SiC and SiO_2 leads an ensemble of P_{bc} -centers with different local geometries subjected to varying strain. The resulting spectrum is hence a superposition of shifted spectra with an already broad intrinsic line shape (cf. Fig. 4). Furthermore, Kimoto *et al.* [24] suggested that the known defect EH6/7 ($E_C - 1.55 \text{ eV}$) could

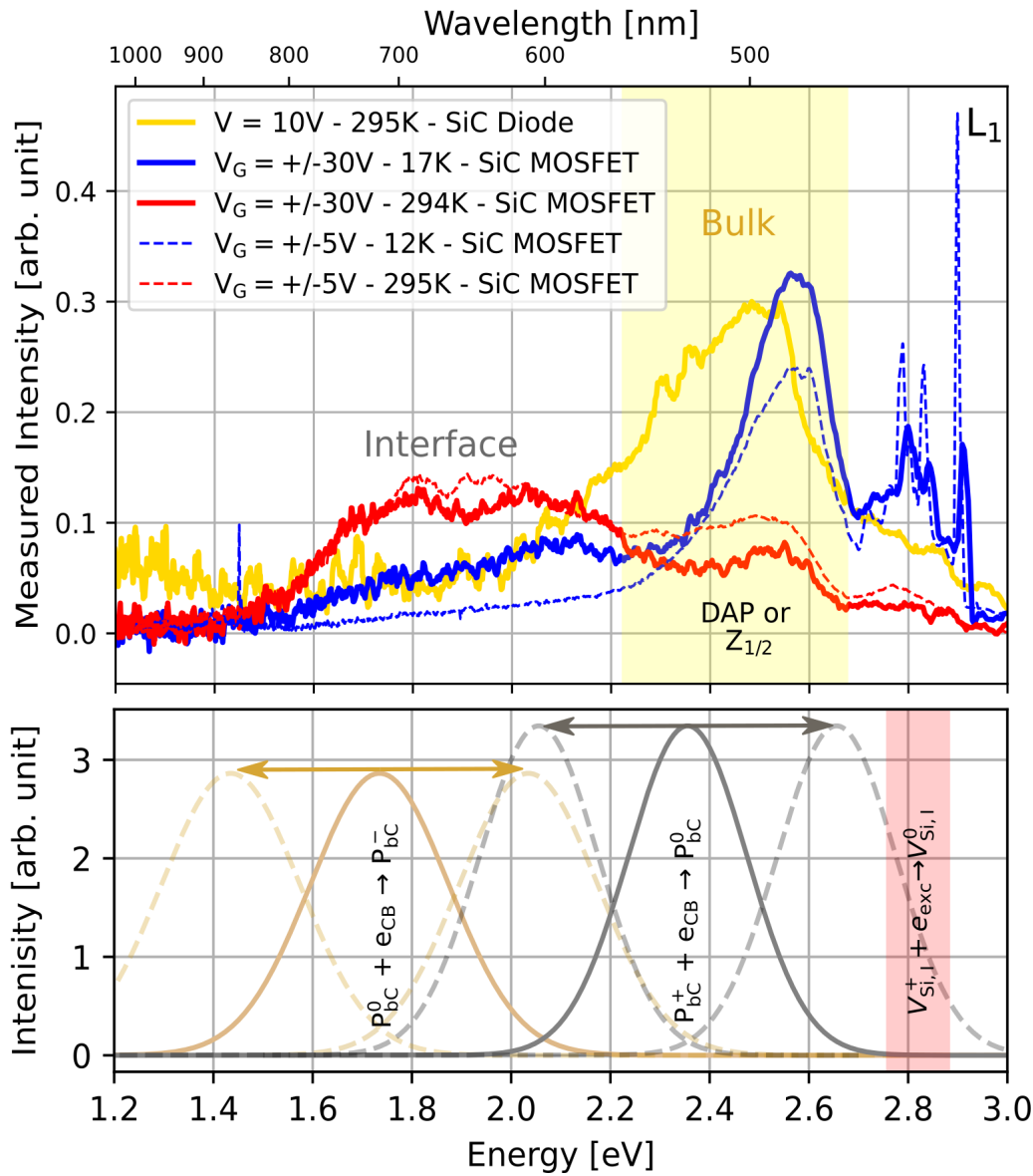


Fig. 4: Recorded spectra of electroluminescence measurements from a pulsed MOSFET test structure at cryogenic and room temperature and the spectrum of a different SiC diode biased in forward direction at room temperature. The amplitude of the gate voltage pulse was varied from ± 5 V to ± 30 V. One can observe a broad peak at 1.8 eV and a second peak around 2.5 eV, that might originate from the bulk. The most pronounced peak at cryogenic temperatures at 2.9 eV is attributed to the L_1 line of the D_1 center [12, 13, 14, 15, 16]. Tab. 1 summarizes the peaks mentioned in literature that might correlate with our measurement. Below, broad emission lines are shown, that are calculated with ab initio calculations. The transitions of the P_{bc} center and the silicon vacancy $V_{Si,I}$ might explain the measured peaks at 1.8 eV, 2.5 eV and 2.8 eV. Calculated transition energies may shift by 0.3 eV due to the variation of the local geometry and the strain at the SiC/SiO₂-interface.

be involved in the recombination process as the emitted photons should have an energy of 1.71 eV. Photon emission around 1.8 eV has also been reported in earlier work [21, 23, 29] measuring thermal stimulated luminescence (TSL) and photoluminescence attributing it to aluminum (Al) as a hole trap or the P_{bc} center. A red-shift in all peaks is observed due to the reduction of the bandgap energy as the temperature increases [30].

Table 1: References found in literature for the peaks at 1.8 eV, 2.5 eV, 2.8 eV and 2.9 eV. Different luminescence measurements methods (L) such as photoluminescence (PL), photoexcitation (PE), thermally stimulated luminescence (TSL), thermoluminescence (TL), electroluminescence (EL), cathodoluminescence (CL) and photo stimulated tunneling (PST) are used.

Peak [eV]	L	Source	Classification
1.82	PL	[29]	O-band / O-defect
1.8	PE	[31]	P_{bc} -/0
1.8	TSL	[23]	Al as hole trap
1.77	TL	[21]	related to Al or B and following recombination
2.554	EL	[17]	defect electroluminescence (DEL) via N and the i-center
2.583	EL	[18]	fast processes of trap filling and free-carrier recombination
2.455	EL	[19]	EK2 donor - D acceptor transition
2.455	PL	[16]	DAP transition
2.6	EL	[32]	radiative recombination involving the HK1 deep center
2.557	EL	[20]	recombination via $Z_{1/2}$ (E_C -0.63eV)
2.583	CL	[22]	DAP (N and Al/B) or recombination via $Z_{1/2}$
2.750	CL	[27]	oxygen related emission
2.77	PST	[1]	intrinsic SiO_2 defect
2.9	PL	[14],[...]	L_1 line of D_1 center

Comparison Between Measurement and Ab Initio Calculations

Our modeling of near-interface recombination centers shows that recombinations of P_{bc} and $V_{Si,I}$ contributes to broad and sharp peaks in the spectral region between 1.5 eV and 2.8 eV. As shown in the bottom pannel of Fig. 4 the measured peaks between 1.8 eV and 2.5 eV, earlier related to donor acceptor pair recombination, could be explained by the P_{bc} -center. The calculated spectrum for the recombination $P_{bc0}^0 + e_{CB} \rightarrow P_{bc0}^-$ is in good agreement with the measured peak around 1.8 eV. The electroluminescence around 2.5 eV coincides with calculated broad recombination lines $P_{bc0}^+ + e_{CB} \rightarrow P_{bc0}^0$, so that recombination via P_{bc} also contributes to the spectral region with bulk-like transitions in the spectrum of a different SiC diode. Note that we only considered one realization of the P_{bc} -center here. At the rough SiC/ SiO_2 -interface an ensemble of P_{bc} -centers with different local configuration exposed to varying amount of strain is present. Hence, the recombination energy can vary by about 0.3 eV. The P_{bc} -center was identified in earlier studies with a spin resonance center at the interface, therefore we suggest this center as an explanation for the peak at 1.8 eV. The calculated transition of $V_{Si,I}$ at 2.82 eV arises from the radiative recombination of an electron trapped in an excitonic state ($V_{Si,I}^+ + e_{exc} \rightarrow V_{Si,I}^0$). This sharp transition has a negligible Franck-Condon shift and may explain the recombination peak at 2.8 eV. Recombination at $V_{Si,I}$ and $V_C C_{Si,I}$ mainly contribute to broad electroluminescence lines in the spectral region below 1.5 eV and are not shown here.

Summary

The electroluminescence spectra of a 4H-SiC MOSFET test structure pulsed at $V_G = \pm 5$ V and $V_G = \pm 30$ V were measured at room and cryogenic temperatures. The spectra change with temperature and gate voltage pulse. The results presented here support the previous assignments of the broad features around 2.5 eV as SiC bulk defects ($Z_{1/2}$ center and others). The peaks at 2.8 eV typically assigned to intrinsic SiO₂ defects have been shown to have a contribution from $V_{Si,I}$. Finally, the peaks at 1.7 eV–2.1 eV can be attributed to interface defects with the P_{bC} (0/-) center at 1.8 eV. A very sharp peak at 2.9 eV, that only appears at very low temperatures, stems from the L_1 line of the D_1 center. Ab initio calculations suggest the P_{bC} center to be responsible for peaks at 1.8 eV and 2.4 eV. The silicon vacancy $V_{Si,I}$ should explain the peak at 2.8 eV.

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