

---

# **BORON DOPED SILICON**

---

## **Author**

Joseph Panama Vera

Material Science of Semiconductors

University of Oslo

May 15, 2024

# Contents

<b>1</b>	<b>Introduction</b>	<b>3</b>
<b>2</b>	<b>Silicon: Description</b>	<b>3</b>
<b>3</b>	<b>Doping silicon</b>	<b>4</b>
3.1	Atomic configurations . . . . .	5
3.2	Electronic properties . . . . .	7
<b>4</b>	<b>Diffusion mechanism</b>	<b>8</b>
<b>5</b>	<b>Boron doping methods</b>	<b>9</b>

# 1 Introduction

Currently silicon is the heart of the electronic industry, due to its versatile semiconductor properties. These properties allow us to control the flows of electrical current. It is also a good material to be doped with impurities, allowing us to create n-type and p-type materials.

In this work the material will be studied using impurities (defects). It will be included cases such as interstitials and substitutionals using boron atom. Besides will be parsed their atomic configurations and electronic properties.

Other important topics to study will be the diffusion mechanism and some practical methods for doping with boron.

## 2 Silicon: Description

Silicon is a type of zincblende structure such as diamond, silicon carbide and cubic boron nitride (Figure 1). This material is a metalloid or semi-metal. Silicon atom have 4 valence electrons and their electronic configuration is given by  $1s^22s^22p^63s^23p^2$ .

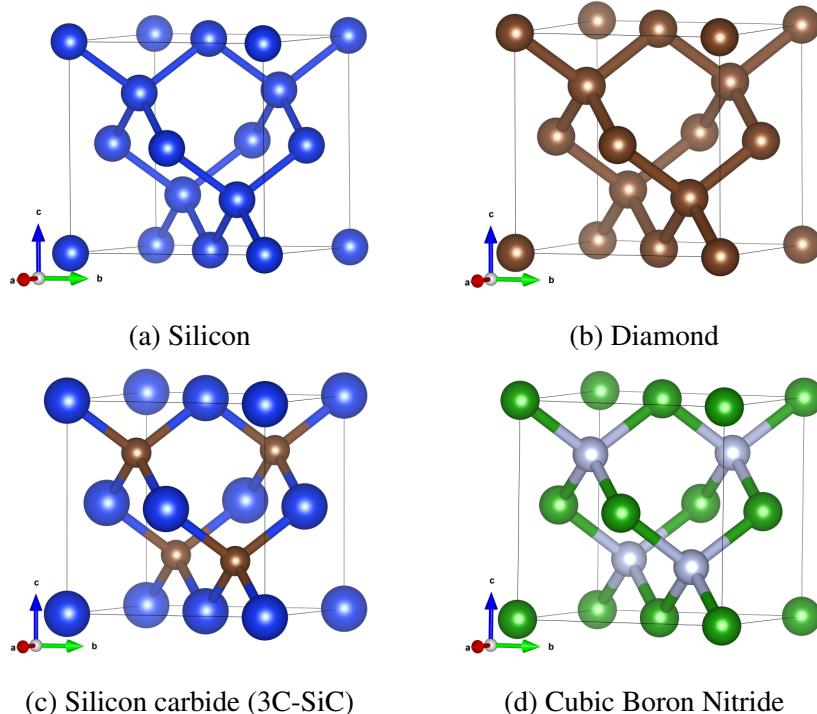


Figure 1: Materials with same structure (conventional cell).

Herein the lattice parameters for conventional cell are given by Table 1.

Table 1: Lattice parameters

Constants (Å)	Angles	Volume (Å <sup>3</sup> )
a = 5.44	$\alpha = 90^\circ$	161.32
b = 5.44	$\beta = 90^\circ$	
c = 5.44	$\gamma = 90^\circ$	

### 3 Doping silicon

In this section, silicon will be doped with boron in different ways (positions).

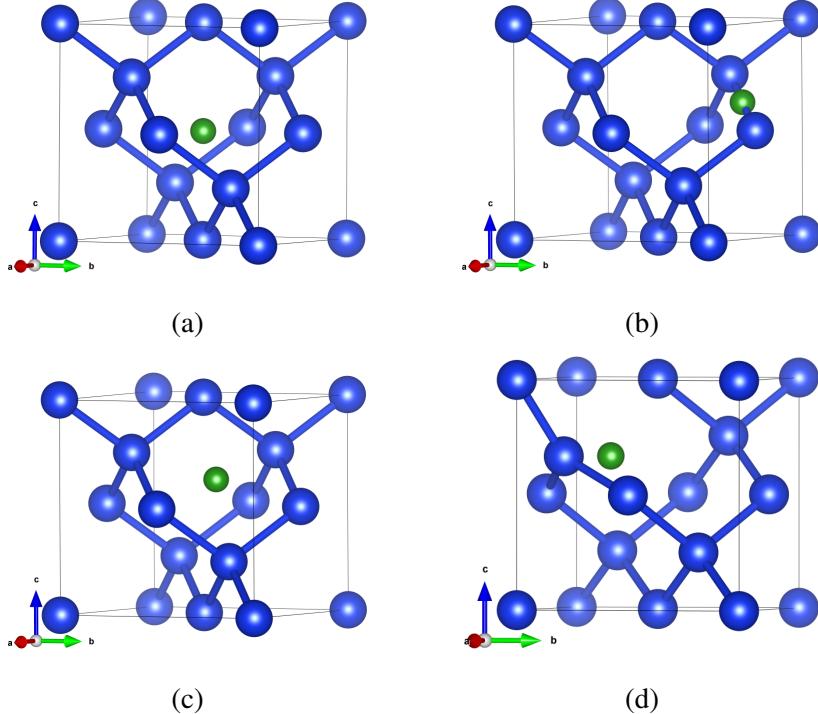


Figure 2: Defects in silicon. (a) Silicon atom is replaced by boron atom ( $B_{Si}$ ) in the center, (b) Interstitial boron in position (0.44,0.56,0.44), (c) Interstitial boron in position (0.56,0.56,0.31), and (d) Silicon atom is moved to (0.46,0.79,0.79), while boron atom is in (0.46,0.71,0.71).

For study impurities or points defects in the materials and get good information about their behaviour, we must to work with supercells. Following previous examples [1], We have used a supercell 2x2x2 with 64 atoms for the DFT (Density functional theory) calculations. Note that Figure 2 is a representation of the supercells and the positions belong to those supercells, images can be seen in the [repository](#).

### 3.1 Atomic configurations

In this section we will study the behavior of electrons and how they are paired. For silicon, this behavior can be divided in N- and P-type semiconductors.

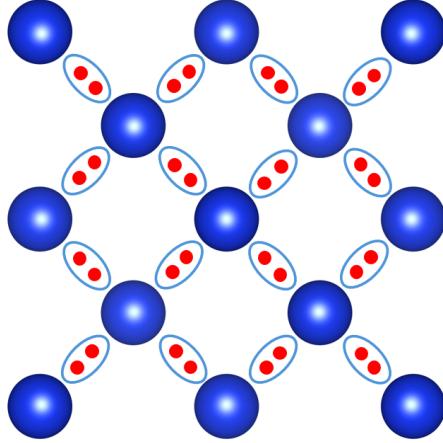


Figure 3: Pure silicon

Figure 3 describes the configuration for silicon without defects, the electrons are paired in normal way. Here the contribution of electrons from each silicon atoms is represented by red balls.

In Figure 4 (a) and (d), the boron atom only have three valence electrons to provide (green balls), so a void will be created. This void will filled with an electron, which will leave a hole (Figure 5). This hole will behaves like a positive charge. This configuration will be referred to as P-type semiconductors, where the majority charge carriers are holes. Next figures (Figure 4 (b) and (c)) the behavior is different, now the electrons unpaired is due to excess electrons, which are provided by the boron. This materials are N-type semiconductors, since the majority charge carriers are electrons. This phenomenon can be seen with the charge density.

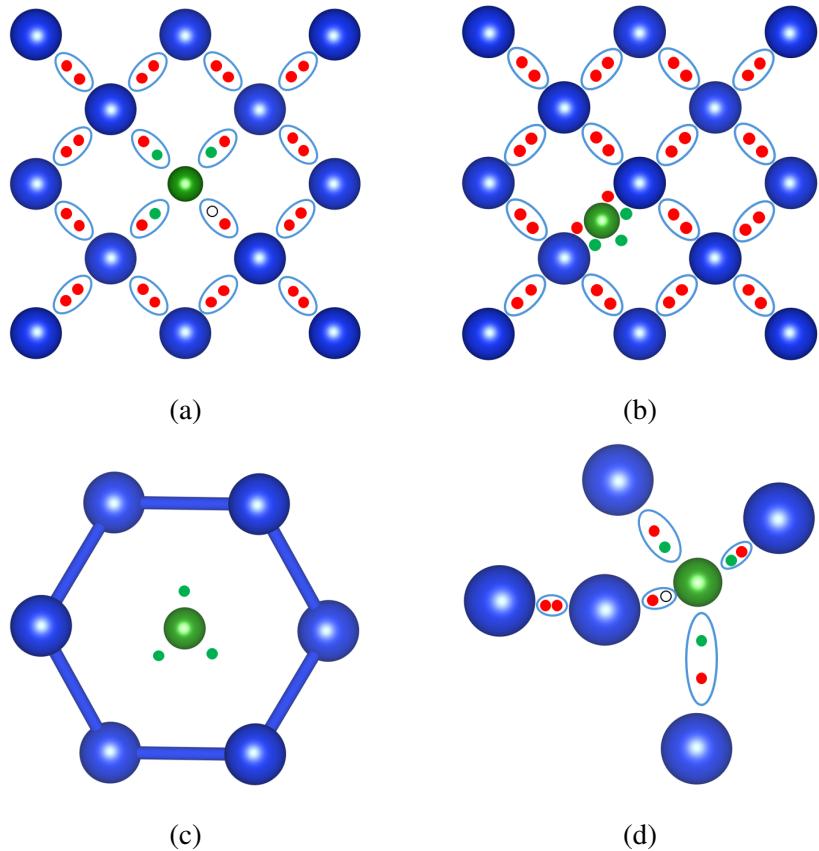


Figure 4: (a)  $B_{Si}$  show us a void or electron unpaired, (b) Interstitial boron in position  $(0.44, 0.56, 0.44)$  have one electron unpaired, (c) Interstitial boron in position  $(0.56, 0.56, 0.31)$  have three electrons unpaired and (d) Boron atom in  $(0.46, 0.71, 0.71)$  have one electron unpaired.

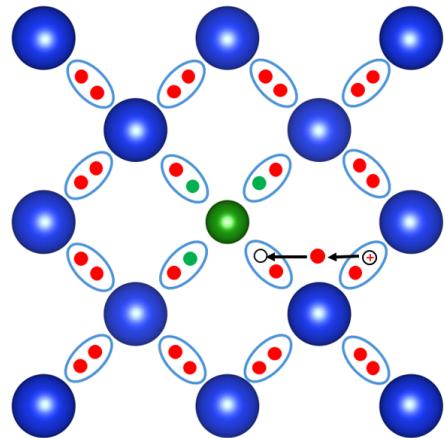


Figure 5: Silicon doped with boron

In strict cases where a silicon atom is replaced by an atom with three valence electrons (group

III elements) or five valence electrons (group V elements) will behave either P- or N-type semiconductors, a clear example is Figure 4 (a).

Instead, interstitial cases should be analyzed according to position like Figure 4 (b), (c) and (d).

### 3.2 Electronic properties

In boron doped silicon with a P-type behavior, the holes can be occupied at low-energy by electrons from the valence band, this means that the acceptor energy level is close to the valence band (Figure 6 (a)), while to N-type behavior the donor energy level is close to the conduction band, the band gap to overcome will be very small (Figure 6 (b)).

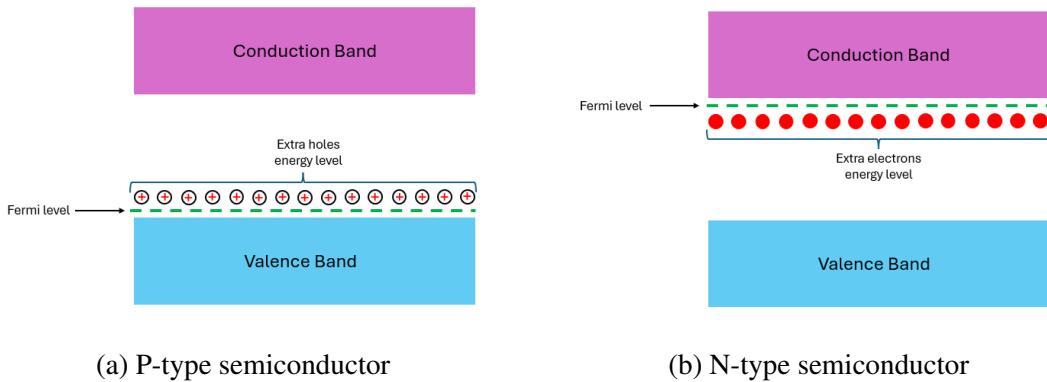


Figure 6: Band structure for doped silicon.

The band structures have been calculated for the examples shown in Figure 1 (a) and Figure 2 using PBE pseudopotential and VASP package, we can see the information in Figure 7 and Figure 8.

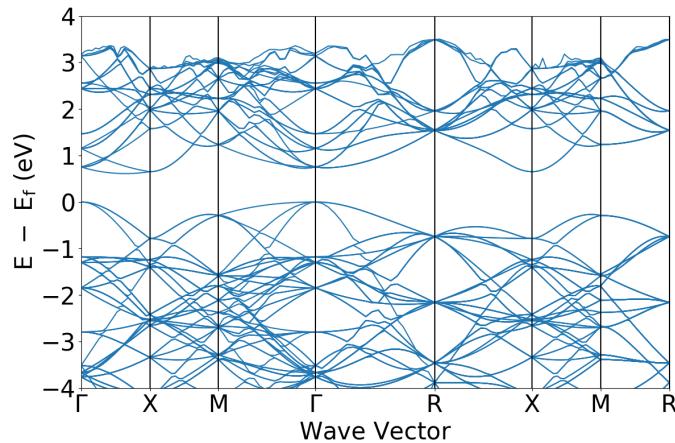


Figure 7: Band structure for pure silicon

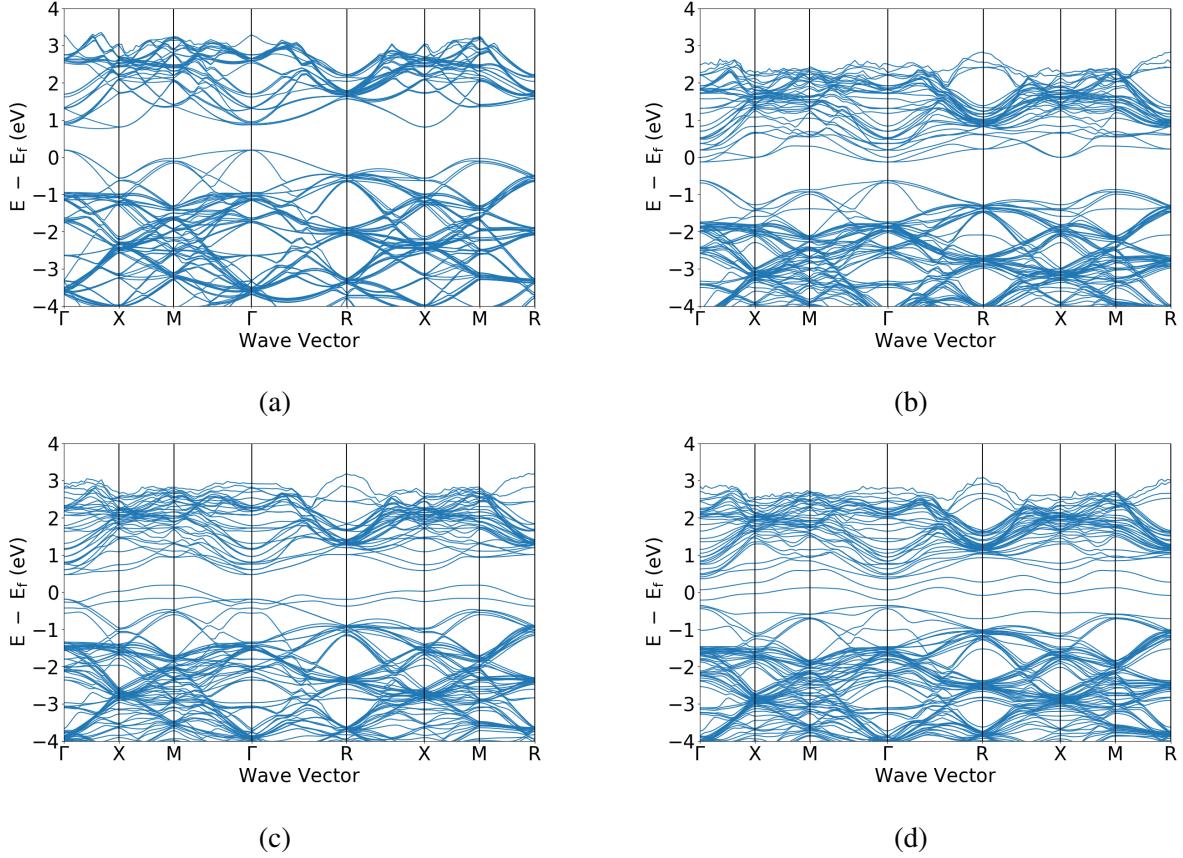


Figure 8: Band structures. (a)  $B_{Si}$ , (b) Interstitial boron in position (0.44,0.56,0.44), (c) Interstitial boron in position (0.56,0.56,0.31), and (d) Boron atom in (0.46,0.71,0.71).

Paths for different structures have a standard definition [2].

## 4 Diffusion mechanism

A basic description is defined as the atomic movement of dopant in the lattice, that means dopant atoms will diffuse from a high-concentration region toward a low-concentration region, which can be explained by Fick's first law. Through this phenomenon, we can get different possibilities either interstitial or substitutional positions into silicon bulk. The distribution of impurities depends on the result we want to obtain, either intentional or unintentional distribution [3].

The results can be vacancies, interstitials or a combination called interstitialcy. This may occur due to high temperature, the atoms vibrate around the equilibrium position with which there is a probability that a atom acquire sufficient energy to leave their initial position and exchange their position with a neighbor vacancy, this case requires a prior vacancy as in Figure 9 (a).

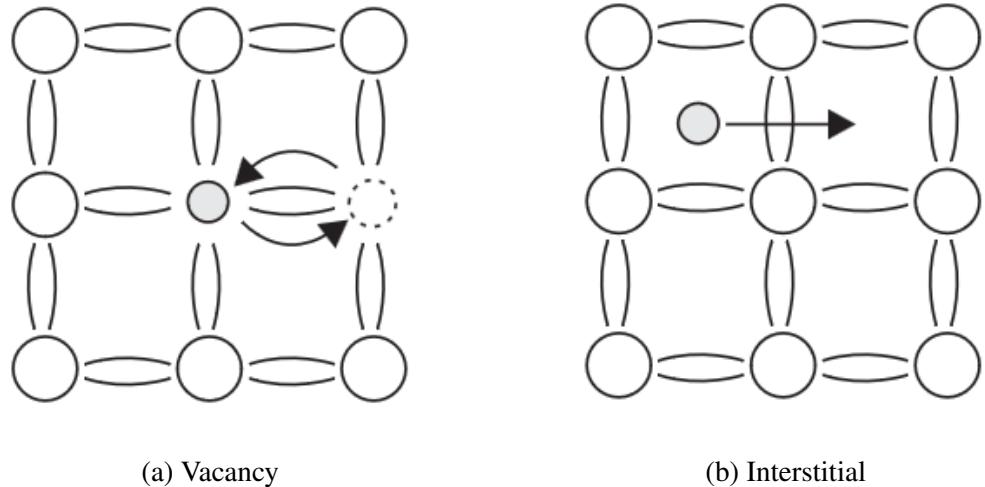


Figure 9: Diffusion mechanisms. Taken from [3].

Interstitial mechanism is due to the movement of the impurity through interstitials position, that means without occupying a lattice site (Figure 9 (b)).

The last case, interstitialcy mechanism also require a prior silicon self-interstitials, herein the silicon self-interstitials moves the impurity to an interstitial position (Figure 10). It can also be used to moves impurities to a lattice site.

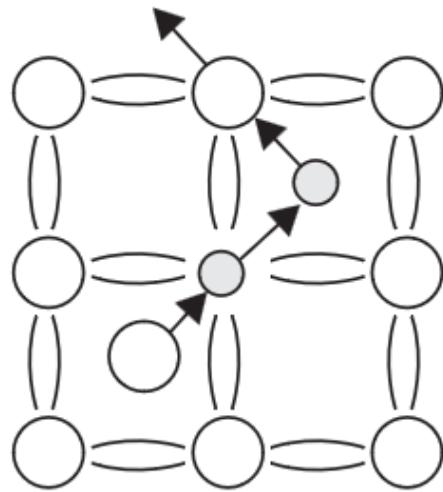


Figure 10: Interstitialcy mechanism. Taken from [3].

## 5 Boron doping methods

In this section will be describes some methods for doping silicon with boron:

- **Ion implantation:** It is currently the most popular method, because is pretty useful. This method is a material modification process, in which an impurity (defect) is introduced at low temperature.

To dope with boron, atoms must be ionized into cations, which will be injected into solid through their acceleration by an intense electric field. This method allows us to reach hundreds of nanometers in depth [4].

The workflow can be seen in Figure 11.

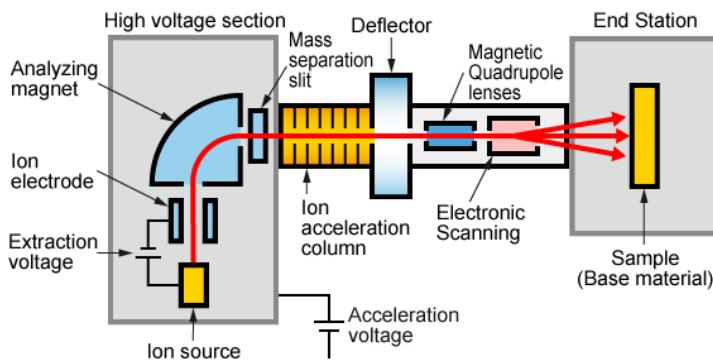


Figure 11: Components of an ion implanter. Taken from [Matsusada Precision](#).

After the implantation is necessary repair the damage created by the ion. The annealing process allow the recrystallization, dopant activation, and diffusion depth.

- **Thermal diffusion:** This method works at high temperature, the dopant atoms are deposited on to or near the surface of the material from the gas phase. When the dopants arrive to the material the maximum concentration is at the surface, therefore exists a concentration gradient between the surface and the bulk, which activate the diffusion. This phenomenon allows dopants to penetrate the material.

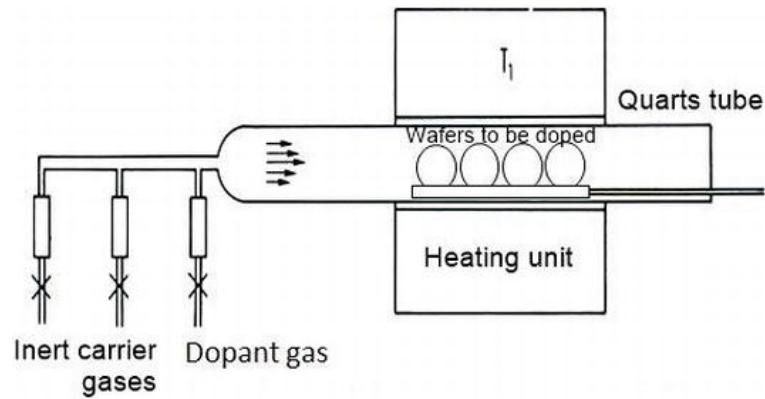


Figure 12: Thermal diffusion method. Taken from [5].

In Figure 12, the inert gas is to minimise contamination.

## References

- [1] Nishimatsu, T., Sluiter, M., Mizuseki,H., Kawazoe, Y., Sato, Y., Miyata, M. & Uehara, M.(2003). Prediction of XPS spectra of silicon self-interstitials with the all-electron mixed-basis method. *Physica B*, 340-342, 570-574. DOI: [10.1016/j.physb.2003.09.133](https://doi.org/10.1016/j.physb.2003.09.133).
- [2] Setyawan, W. & Curtarolo, S. (2010). High-throughput electronic band structure calculations: Challenges and tools. *Comput. Mater. Sci.*, 49(2), 299-312. DOI: [10.1016/j.commatsci.2010.05.010](https://doi.org/10.1016/j.commatsci.2010.05.010).
- [3] Jones, S.W. (2008). Diffusion in Silicon. IC Knowledge LLC.
- [4] Chi T. Cao, L., Hakim, L., & Hsu, S.-H. (2022). Boron Doping in Next-Generation Materials for Semiconductor Device. IntechOpen. DOI: [10.5772/intechopen.106450](https://doi.org/10.5772/intechopen.106450).
- [5] Li, F., & Jennings, M. (2018). Main Differences in Processing Si and SiC Devices. IntechOpen. DOI: [10.5772/intechopen.76293](https://doi.org/10.5772/intechopen.76293).