## Theory of defects in SiC – impact on the sensitivity of radiation detectors

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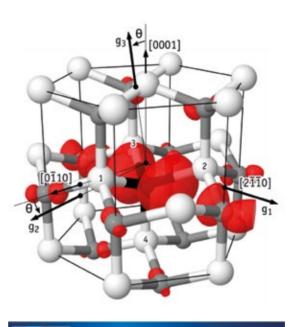
Increasing geopolitical risks have urged a massdeployment of screening systems capable of detecting chemical, biological, radiological and nuclear threats. This is the underlying motivation of E-SiCure2, a project funded by NATO Science for Peace and Security Programme, which joins research teams from Slovenia, Croatia, Japan and Portugal (i3N-Aveiro). The goal is to develop a miniaturized semiconductor structure capable of detecting ionizing radiation, including neutrons, emitted from radiological sources, and of being incorporated into a pixelized device.

Researchers from the Theoretical and Computational Physics group at the i3N-Aveiro have been developing physical models for the excitation, transport, and loss of impact-generated carriers within silicon carbide (SiC), a semiconductor known for withstanding high radiation doses. According to a recent paper published in Physical Review, they found that boron, a contaminant often found in commercial SiC materials, has the properties of a recombination center. Such centers are highly harmful as they attract both electrons and holes, promoting their annihilation, and consequently, leading to the loss of signal during radiation detection.

The work was able to account for a multitude of boronrelated optical, junction, and paramagnetic resonance experiments available in the literature. By describing the motion of thousands of electrons around a boron impurity in SiC (Figure 1), it was concluded that boron is ineffective as a p-type dopant. In n-type SiC, which is the detector-grade material of choice, boron contaminants are negatively charged, are effective traps for impact-generated holes, and therefore are likely to act as strong recombination centers. These results will improve our ability to monitor boron contamination in SiC devices, and ultimately to raise detection sensitivity by fabrication of boron-free SiC.

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## FIGURE 1

Spin-density close to a boron impurity in 4H-SiC. The principal directions of the calculated gyromagnetic tensor are also depicted. This quantity allowed us to unambiguously connect the model with an observed paramagnetic signal, and by that way to monitor and quantify the boron contamination [adapted from Torres et al., Phys. Rev B 106, 224112 (2022); DOI: <u>TO.1103/</u> PhysRevB.106.224112].

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