



Exploring point defects as qubit candidates in cubic boron nitride

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Introduction

Quantum technology (QT) and quantum computing in general have opened a wide world of research in the solid state physics. This new field uses the fundamental principles of quantum mechanics such as superposition and entanglement, which are characteristics of qubits. Currently, the physical platforms to implement qubits are in most cases based on superconducting materials, which operate at cryogenic temperatures (near to absolute zero). The low temperatures are necessary to make sure the qubits are stable with long lifetime or coherence time. Reaching cryogenic temperatures requires a lot of energy, maybe even more than classical computers. For this reason, it is necessary to look for new quantum materials that operate at ambient temperatures and reduce energy consumption, which can help us combat climate change.

Search for new materials

The main reason to look for new materials is to make qubits in new ways.

- Qubits, based on superconductors, are resource-intensive (energy).

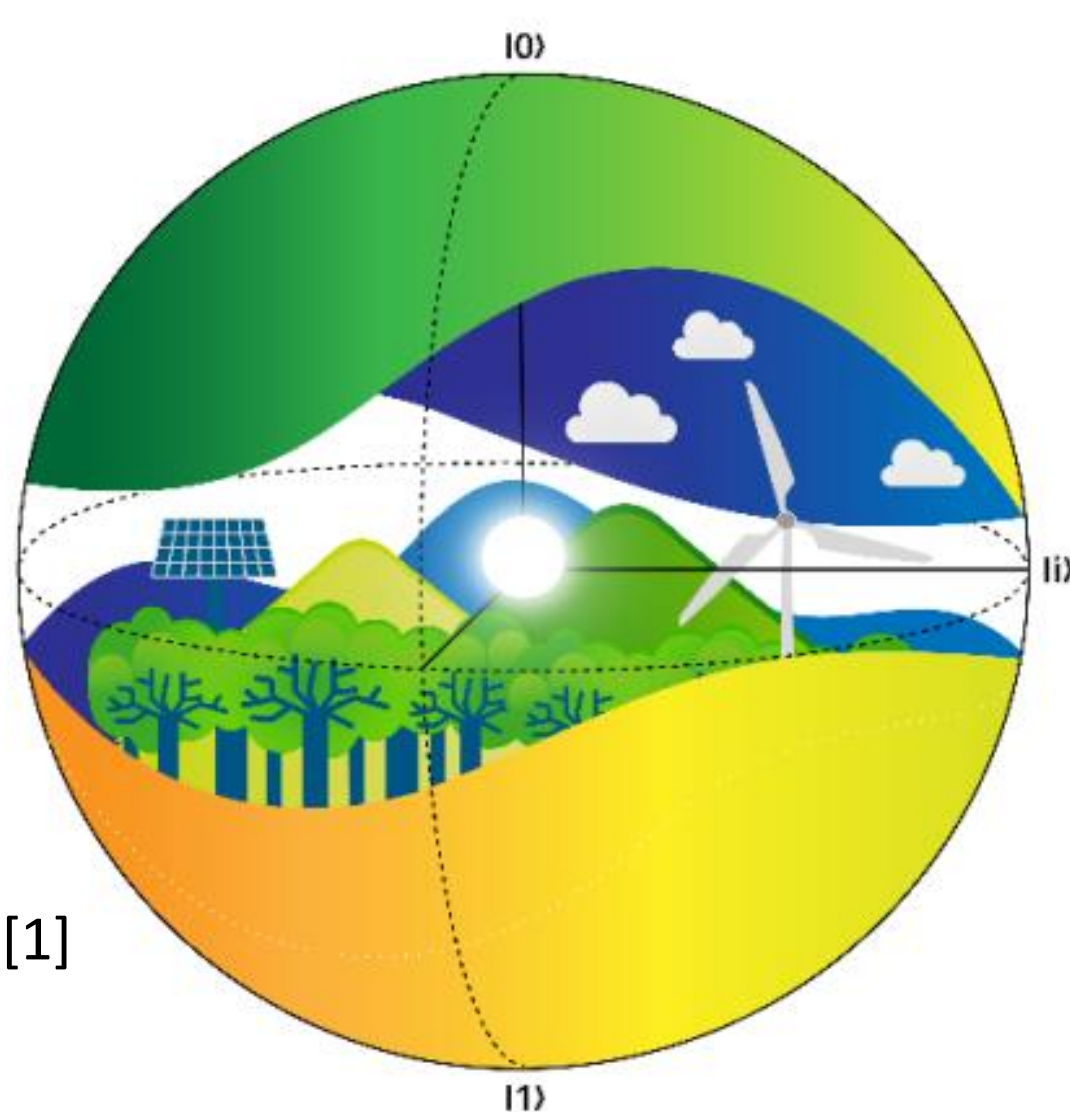


Figure 1: Qubit [1]

- Improved QT platforms also positively affects our relationship with the environment.
- For example, machine learning algorithms can be used to predict the properties of new materials based on their structural features [2].

Impact of quantum computing on sustainability

Solutions and improvements to pollution through carbon capture, the use of renewable energies such as solar, wind and hydraulic energy, and energy storage.

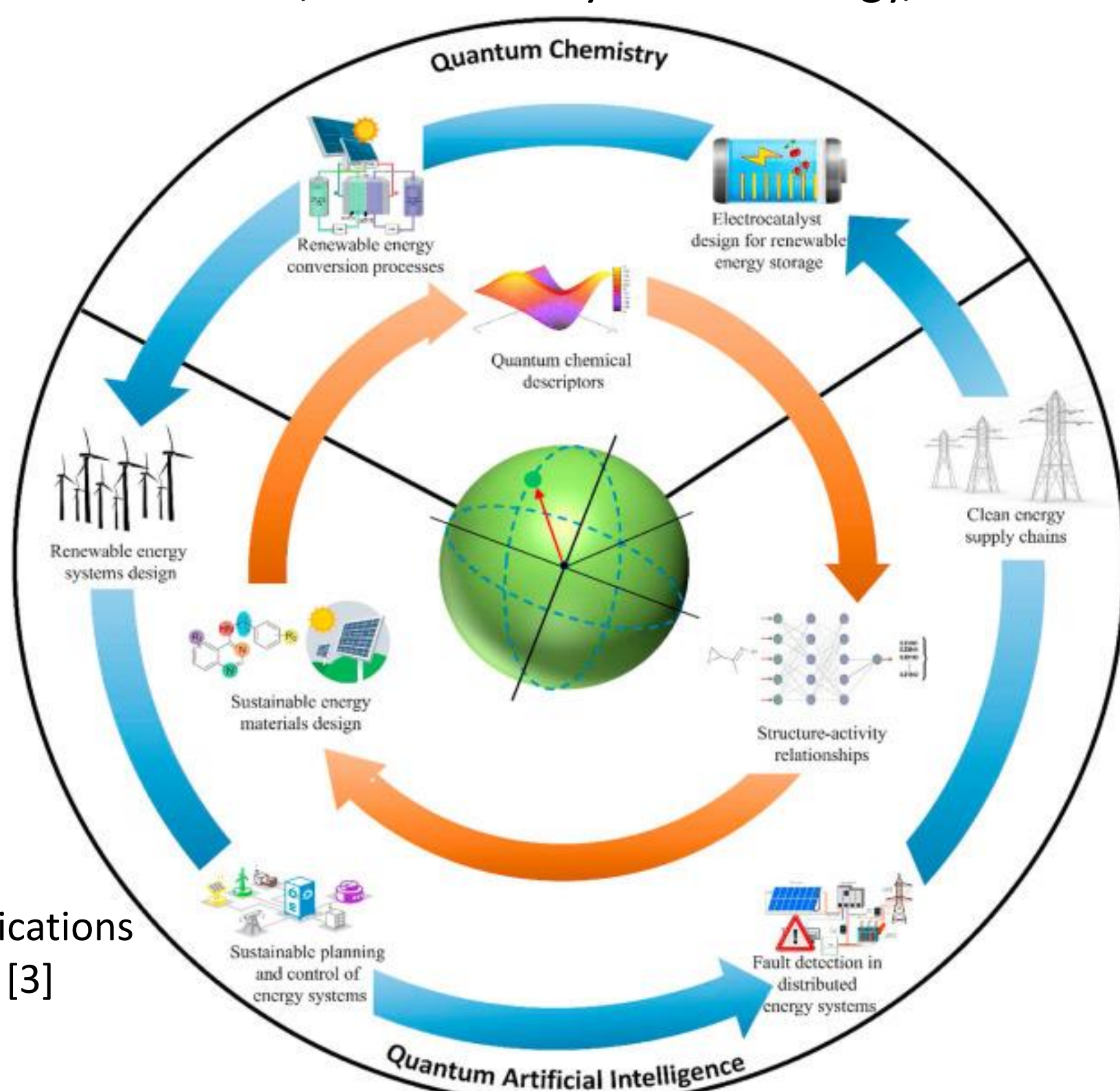


Figure 2: Potential applications of quantum computing [3]

- Simulation of physical systems such as catalysts, batteries and carbon capture materials.
- Optimization to electrical grid and vehicle routing.
- Machine learning to earth system modeling and materials discovery. Quantum computers and quantum sensors are vital in these efforts.



Figure 3: Sustainability [4]

Point defects in cubic boron nitride

- Point defects in semiconductors can be used as spin qubits and single-photon emitters (SPE) for QT.

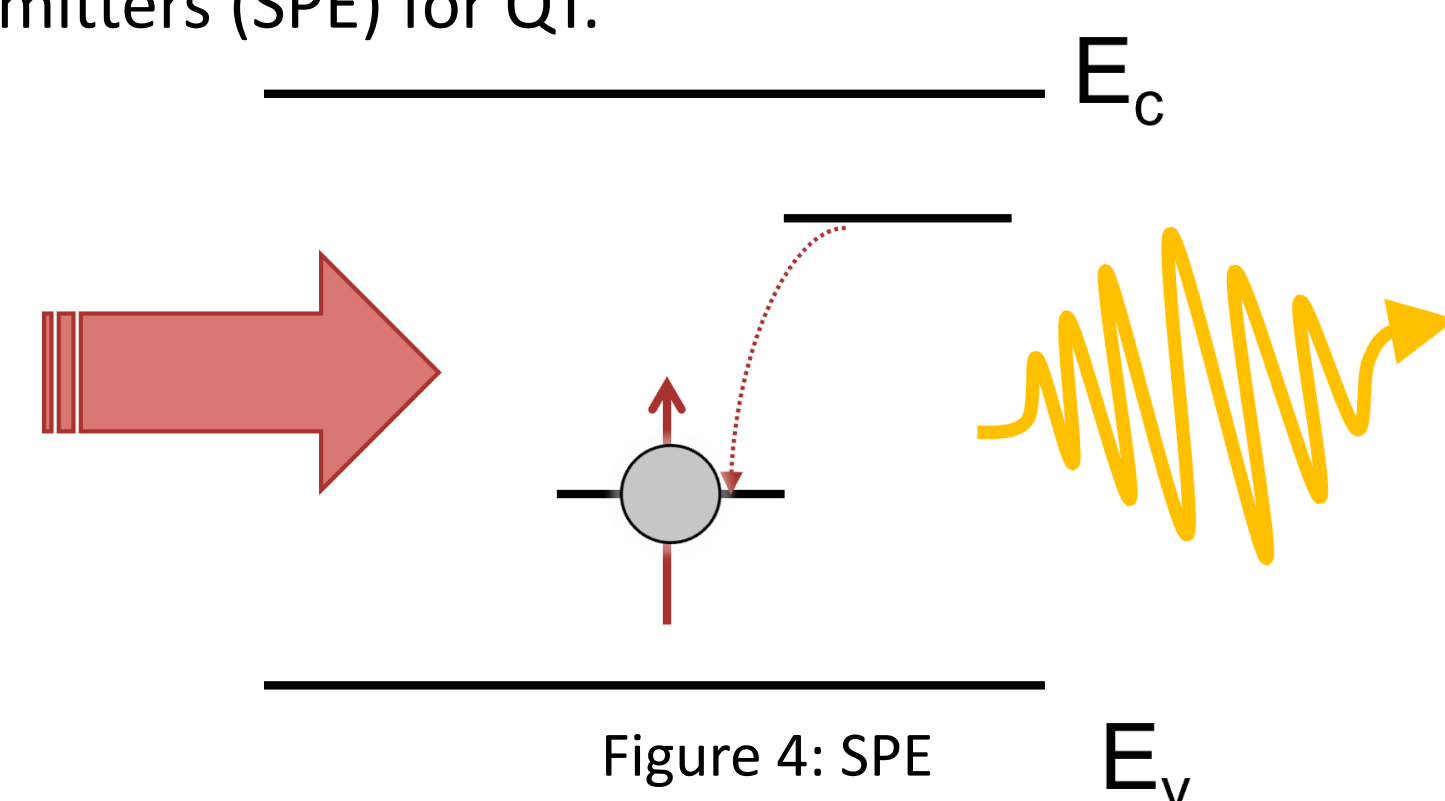


Figure 4: SPE

- Materials like SiC (silicon carbide), Si and hBN (hexagonal boron nitride) have demonstrated, through point defects, to be useful for QT.

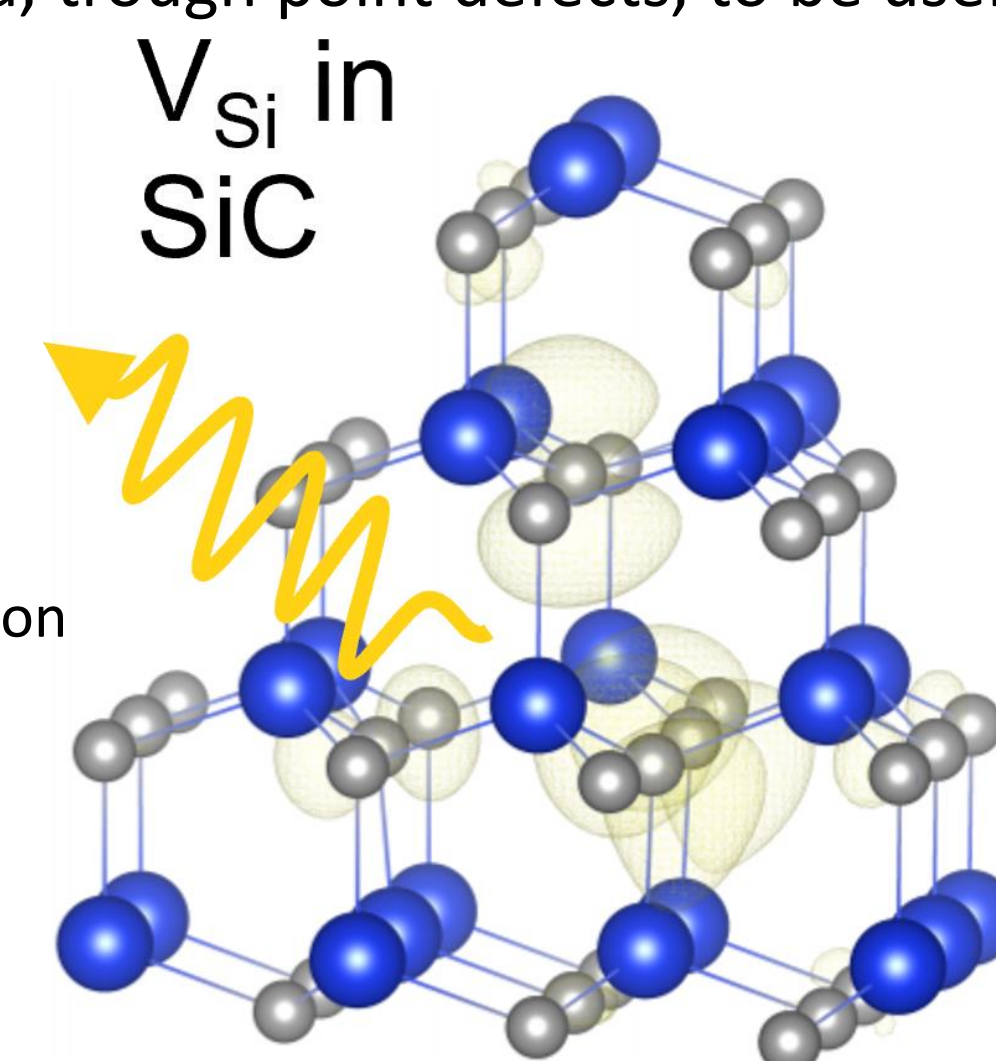


Figure 5: SPE in Silicon Carbide

- In this MSc thesis project, point defects in c-BN will be studied using powerful tools such as first principles theoretical simulations based on density functional theory (DFT).

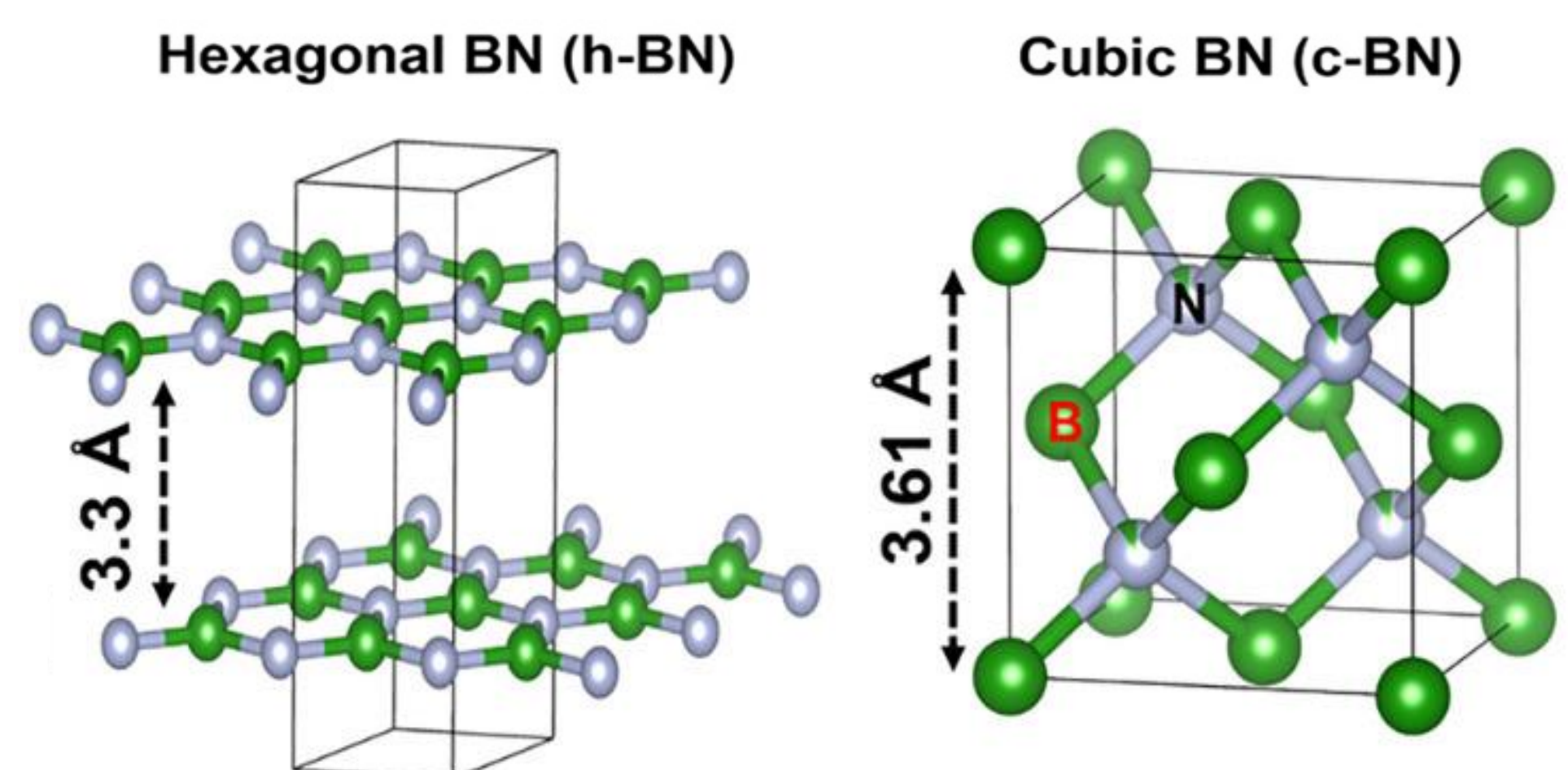


Figure 6: Unit cell [5]

- If we want to take the next step towards the quantum world without compromising our relationship with the environment, we should strive to build quantum computers based on semiconductors.

References

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- [2] Hebnes, O.L., Bathen, M.E. & Schøyen, Ø.S. (2022). Predicting solid state material platforms for quantum technologies. npj Comput. Mater., 207(8), 1-15.
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