The project titled "Determination of the local structure of boron carbide ($B_{13}C_2$) using the Pair Distribution Function method" aims to apply innovative crystallographic methods in studies on the local structure of boron carbide. The Pair Distribution Function (PDF) method allows describing interatomic distances in crystalline material (not exclusively). It is based on powder diffraction (X-Ray or neutron) data but the analysis is performed in real space. This method is primarily utilized for disordered systems, which includes boron carbide $B_{13}C_2$. The mechanical properties of $B_{13}C_2$, such as high hardness (comparable to diamond), thermal stability, and chemical resistance, make it desirable for various technological and industrial applications. Ongoing research is also exploring its potential as a superconducting material or neutron detector.

However, accurately description of this compound structure is challenging due to the similarities between the isotopes ^{11}B and ^{12}C, making it difficult to distinguish between these two atoms using standard diffraction methods. The difficulties in determining the precise atom positions pose a significant problem as disorder and structural defects directly affect the material's mechanical properties. Available publications indicate that theoretical DFT (Density Functional Theory) simulations classify boron carbide as a metallic material, but experimental measurements suggest it behaves as a semiconductor. These discrepancies arise potentially from the disorder present in the structure. Therefore, the aims of this project is to focus on determining the local structure of $B_{12}C_2$, which will be achieved through:

- Synthesizing the compound using the Self-propagating High-temperature Synthesis (SHS) method at different temperatures to evaluate the impact of synthesis temperature on structural defects.;
- Conducting synchrotron X-ray PDF measurements at large scale facilities;
- Analysing the data and applying the Pair Distribution Function (PDF) method;
- Utilizing the Reverse Monte Carlo method to determine the local structure and potentially its level of disorder.

It is important to emphasize that this is a novel approach to addressing the structural description of this compound, which has not been previously utilized. However, my simulations demonstrate that despite the similarities between boron and carbon atoms, it is possible to distinguish and determine exact atomic positions. The outcome of this project will be a description of the material's local structure, highlighting the influence of synthesis temperature on disorder and defects in the crystalline structure of $B_{13}C_2$.