Metallic and semiconductor nanowires (NWs) are being pursued as versatile building blocks for nanoscale electronics. Recent experiments have shown that a variety of functionalities can be built into NWs, which can be doped to serve as active devices while simultaneously serving as interconnects. With the rapid advances in the controlled fabrication of thin NWs, the experimental techniques often reach the limit where they are insufficient for obtaining precise knowledge of the atomic structure. For any given material, however, the structure of a thin NW is the single most important factor that determines its properties and associated physical phenomena, and therefore, warrants intense theoretical investigations.

The aim of this project is to find the structure of boron and boron-related nanowires with diameters smaller than 3 nm. We are interested to study the electronic, magnetic and elastic properties of these nanowires as a function of their diameter. In particular, we will examine (i) "clean" and passivated by hydrogen boron nanowires, (ii) nanowires made of alloys, binary compounds as well as 1D heterostructures, (iii) finally boron nanowires doped with metals (eg. Mg). To achieve our goal, the structure of the nanowires will be found using evolutionary-based search algorithms coupled with first-principles DFT (density functional theory) calculations.

The choice of boron [1] as the material on which we will develop our methodology of searching for the structure of nanowires is not accidental. Like carbon, boron has a very rich chemistry, and thus comes in many allotropic forms. Experimentally is confirmed the existence of 5 of its allotropic forms, although at least 14 more allotropes have been reported. It is therefore, quite natural to expect that also in one dimension boron can have many forms, which have not yet been discovered.

[1] N. S. Hosmane, *Boron Science: New Technologies and Applications* (CRC Press, 2016).