Bachelor thesis project

Density functional theory calculations for Schwarzites structures

Schwarzites (named after the mathematician Hermann Schwartz) are a particularly interesting class of hypothetical carbon-based structures (carbon allotropes) the generalize the combinatorics of tradtional graphene to more complicated ring structures and hence topologies. In this project, the student will utilize density functional theory (DFT) methods to analyze the feasibility of particularly interesting Schwarzites.

DFT is a computational method for analyzing the energetics and electronic structure of e.g. crystalline materials. Schwarzites are often generated using combinatorial methods; in this project we aim to take on a more physics-based perspective of such structures to ascertain their feasibility as actual physical structures one might expect to be able to synthesize.

On a practical level, the student will get familiarized with the software QuantumEspresso to analyse selected, particularly interesting reticular structures from the RCSR database (or possibly the ToposPro database).

The student will get hands-on experience with:

- The theory behind DFT
- Carbon allotrope structures and their crystallography
- Combinatorics and mathematics of reticular structures
- High-performance computing methods

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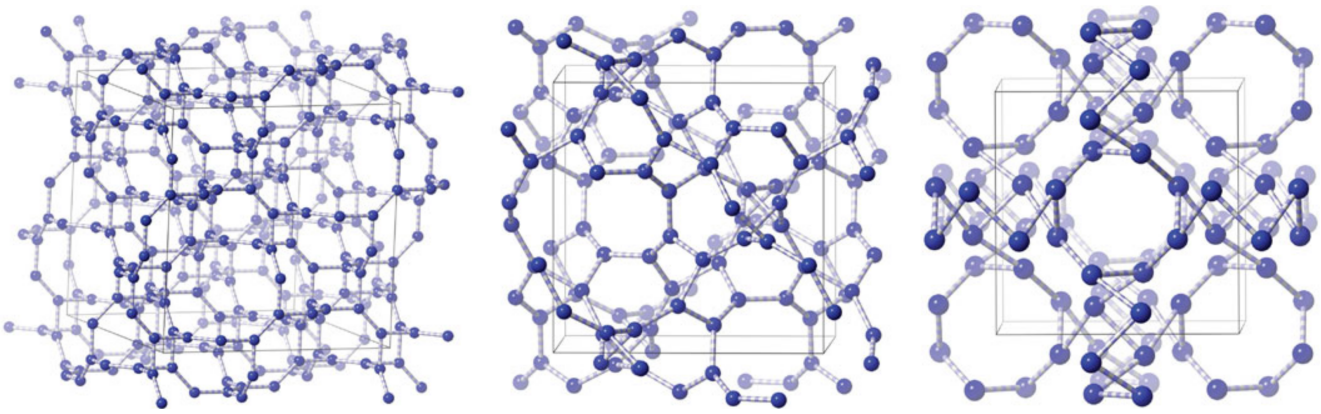

Figure 1: Three examples of Schwarzite crystal structures. Each blue sphere represents an sp^2-conjugated carbon atom. The unit cells are shown in black outline.