Influence of boron and nitrogen dopants on electronic and transport properties of graphene and graphyne nanoribbons

It is challenging to find an adequate semi-conducting replacement for silicon in post-silicon electronic devices as in the field-effect transistors. The basic prerequisite for this application is the existence of the band gap which would enable the device to be switched between the off and on states. One of the most promising choices is graphene due to its outstanding properties such as flexibility, resistivity, chemical stability and high electrical and thermal conductivity [1-5] but the lack of an energy gap is the obstacle that one has to confront. Electronic and transport properties of graphene-like materials can be enhanced by introducing structural defects or by chemical doping [6,7]. The interesting candidates which show the enhancement of these properties and which are precisely experimentally producible are graphene nanoribbons [10,11] and graphynes - the family of graphene allotropes [12,13]. For chemical doping, the ideal candidates are boron and nitrogen [8,9] (as well as the radical groups that contain them) due to their dimensional and electronic similarities with carbon.

The outcome of this thesis will be the analysis and comparison of the electronic and transport properties of the graphene nanoribbons with edges of different shapes (armchair, zigzag and chiral) and analogous chosen structures from the graphyne family, and the effect of introduced dopants on their properties. The calculations will be performed using *PyBinding* and *Kwant Python* packages for numerical tight-binding calculations. For the preparation of this thesis, the basic knowledge of quantum and solid-state physics is required as well as some programming skills in *Python*.

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