This proposal is devoted to the theoretical investigations of the electronic and magnetic structure of two-dimensional (2D) systems based on boron and boron-related compounds. Various parameters of the studied materials can be tuned, enabling controlled and reversible access to a diverse set of quantum phases. The study of novel materials with unique electronic and magnetic properties constitutes the most attractive branch of contemporary solid-state physics. An example of such a system is a Dirac material in which the dynamics of electrons is described by the Dirac equation instead of the Schrödinger one. In this case, the relativistic mass of fermions can be zero, leading to the linear dispersion relation (so-called Dirac cones in the k-space). These types of materials are represented by a rich range of so-called topological materials, e.g., topological insulators (TIs), topological semi-metals (TSMs), and topological superconductors (TSs) with considerable potential for applications in the various fields. Besides device applications, these systems are expected to realize such elusive phenomena as magnetic monopoles or Majorana fermions. However, such accomplishments require the possibility of manipulating the electronic and magnetic structure of topological materials.

The main purpose of this proposal is to search for two-dimensional topological insulators with large bandgaps and the first theoretical realization of a monoatomic 2D nodal line semimetal. To achieve this goal three factors have to be considered in the prospective systems. First, the candidate 2D materials have to be simple in their structure and previously reported as possible 2D TIs by theoretical investigations [1]. Second, the 2D structures have to be accessible from the point of view of the experimental growth. Finally, since the studied quantum phenomena are rather complex, we give preference to these 2D materials with which we have had some theoretical experience before [2]. The materials in question are 2D forms of boron called borophenes. Although similar to graphene in its lightweight nature and strength, borophene has distinguishing features that contribute to its novel desirable properties. The most important is its structure which consists of a highly variable boron atom network of hollow hexagons (vacancies) in a reference hexagonal lattice. By tuning the vacancy concentration, we can tailor its electronic and mechanical properties [3].

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