Computational materials discovery in various dimensionalities

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Nowadays one of the most developing fields of science is the investigation of physical and chemical properties of materials of various dimensions. The study of low-dimensional nanostructures is mainly related to the study of ultrathin monoatomic layers of various compositions. Among the latter, particular attention is drawn to such films of atomic thickness as graphene, its derivatives. In addition, many of non-carbon materials, which has no layered counterparts in bulk, are found to be layered graphitic-like in nanoscale. Such evidences related to silicon carbide, zinc oxide and aluminum nitride. Using modern methods of computational materials science, we provided the comprehensive investigations of ultrathin carbon films with nanometer thickness along with freestanding films of ionic compounds.

In the field of bulk materials (single crystals, composites, etc.), the main direction of theoretical material science is search for crystal structure with optimal desired properties, such as hardness, band gap, dielectric constant, etc. Using the evolutionary algorithm implemented in the software package USPEX, it became possible to predict stable compounds, their crystal structure using only data on their chemical composition. We studied the phase diagram of Cr-C, Cr-B, Cr-N systems to find the hardest possible materials among all possible phases. Among predicted Cr-N phases several high energy density materials were predicted showing nitrogen polymerization at ~15 GPa.