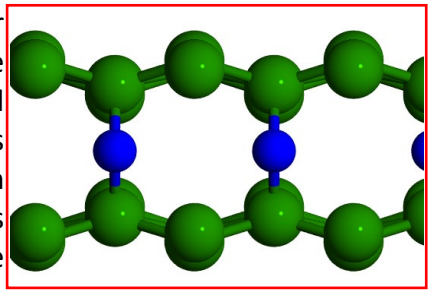
Hydrogen-induced superconductivity in bilayer borophene structures

Placed between metals and non-metals in the periodic table of elements, boron is one of the most chemically flexible atoms, forming different kind of bulk polymorphs, originated from the electron deficiency, resulting in the multicenter B–B bonds, which are much more complicated than those of carbon **[1]**. Broad studies on small-scale planar boron clusters provided, in 2015, the first experimental evidence for the growth of two-dimensional (2D) boron structures, named borophenes **[2]**. The novel properties of borophenes, such as mechanical compliance **[3,4]**, optical transparency **[5]**, ultrahigh thermal conductance **[6]**, the presence of metallic Dirac fermions **[7]**, and superconductivity **[8,9]**, have attracted intensive theoretical and experimental interest.



In addition to monolayer, single-crystalline β_{12}-like bilayer borophene, with zig-zag rows, was synthesized on the Cu(111) surface by molecular beam epitaxy **[10]**, opening the question of whether stable bilayer structure of usual borophene sheets can exist. Several theoretical calculations indicate significant stability of such freestanding bilayer structures **[11,12]**, with interesting superconducting properties **[13]**. Another very promising and interesting way of getting phonon-mediated superconductors is by using different intercalated elements within bilayer borophenes **[14,15]**.

In this work, we will focus on advantageous way to strongly enhance phonon-mediated superconductivity in bilayer borophene structures by adding hydrogen atom(s), analyzing the changes in the structural, electronic and vibrational properties that hydrogen atom(s) will induce in such systems, and which will be, hopefully, satisfactory for this type of research. Our motivation for this kind of work is based on the fact that hydrogen-induced 2D superconductivity, with very high critical temperature, has been realized in a diverse range of materials. Detailed and precise *ab-initio* description of such H-doped bilayer boron systems will be needed in order to obtain appropriate input parameters for phonon calculations using DFPT method together with anisotropic Migdal-Eliashberg formalism.

During the research, the candidate will also have the opportunity to get acquainted with various software packages and graphical programs specialized for this kind of theoretical research of nano-superconducting materials.

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