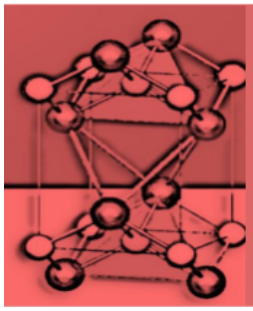

X Workshop on Novel Methods for Electronic Structure Calculations

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A new 2D chemistry of Boron?

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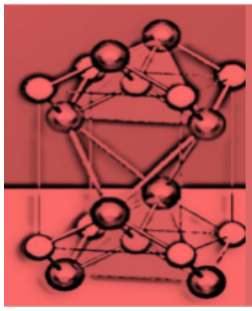
The isolation of a 2D hexagonal borane layer $(BH)_1$ – borophane – from superconducting MgB_2 [1] and the 2D hexagonal pure boron layer β_{12}-borophene [2,3] calls for the possibility of developing a new 2D boron chemistry.

In the same way as benzene C_6H_6, discovered by Faraday back in 1825 as an aromatic transparent liquid [4], is the repetitive pattern in 2D graphene, planar cyclohexaborane(12) B_6H_{12} with D_{3h} symmetry, a yet unknown molecule, is the repetitive pattern in borophane. Hexaborane(12) B_6H_{12} is a (3D) non-planar concave open polyhedral molecule with C_2 symmetry; this molecule exists and is also a transparent liquid that, like most boron hydrides, is readily hydrolyzed and flammable. We have proved, by means of quantum-chemical computations, that a $3D \rightarrow 2D$ isomerization of hexaborane(12) to planar cyclohexaborane(12) is feasible [5] and fully rationalizable in terms of newly developed conceptual tools [6]. Similarly, there is a one-to-one correspondence between any planar or non-planar open or polycyclic conjugated hydrocarbon and the corresponding borane: $C_nH_m \longleftrightarrow B_nH_{m+n}$ [7,8]. The problem is that until now the only known correspondence is between ethylene and diborane(6): $C_2H_4 \longleftrightarrow B_2H_6$. The purpose of this talk will be the description, by means of electronic structure computations, of potential new planar borane molecules and their properties.



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