Abstract

The synthesis of graphene opened a new era in the search for new materials for nanotechnology applications. In this sense, 2D materials with a large surface-to-volume ratio, stability, and excellent electronic, thermal, transport, and mechanical properties are potentially suitable for gas sensing, chemical adsorption, and catalytic applications.
Belonging to the same family of two-dimensional mono-elemental materials, Xenes (where X represents the constitutive element), borophene, composed exclusively of boron atoms, was first theorized in the 1990s and subsequently synthesized in 2015. Since then, its outstanding physical and electronic properties have been recognized, although this promising material is still in an early stage of development. In this regard, a theoretical analysis of its properties and applications can become a starting point for further experimental research.
Boron, the metalloid element with an electronic configuration $1s^2 2s^2 2p^1$ is electron deficient. This electronic condition causes the formation of exotic bonding states, which lead to several polymorphisms, in contrast to its immediate neighbors in the periodic table, carbon and silicon. Interestingly, the corresponding two-dimensional one-atom-thick crystal can be obtained through the growth on a metal substrate such as Ag. Moreover, some studies have revealed that including transition metal atoms can stabilize borophene by electron transfer from the metal to the boron.
In this context, MBenes are two-dimensional materials that derive from their parental MAB bulk phases (where M is a transition metal, A is frequently a group IIIA-IVA element, and B is boron) and are, for this reason, regarded as relatives to MXenes which have drawn tremendous attention in recent years. MBenes exist in several stoichiometries, and the presence of transition metal atoms confers them a special robustness and magnetic properties that open new windows to the boron-based compounds.

This thesis focuses on two different classes of boron-based materials as potential candidates for gas sensing or absorption:

(i) **Specific borophene polymorphs (α-sheet, buckled hexagonal, and honeycomb-like) with diverse structural and physicochemical behavior**: First-principles calculations have been performed in the framework of the Density Functional Theory (DFT), to calculate the influence on the structural, electronic and magnetic properties after the adsorption of hazardous gas molecules (CO, CO_2, NO, NO_2 and NH_3) on the α-sheet, buckled hexagonal, and honeycomb-like borophenes. We have observed that the charge transfer between the molecules and the 2D structure destabilizes the bonds, producing wrinkles, which causes boron to form sp^3 hybridization instead of the sp^2 one present in the flat (or quasi-flat) borophene, a circumstance that leads to a strong bonding with the adsorbate and make this material optimal as gas adsorbent.

(ii) **MBenes with M_2B_2 stoichiometry (M = Cr, Fe, and Zr)**: As a first step in our research, we investigated the properties of pristine MBenes, which revealed their outstanding structural strength and thermal stability as well as good conductivity. Additionally, and due to the presence of transition metal atoms in their composition, we have observed that introducing the Hubbard correction has a non-negligible influence on their electronic and magnetic ground states. Moreover, the results arising from their magnetic properties point to their use as robust magnets with high critical temperatures. From the perspective of the adsorption of both harmful molecules (CO, CO_2, NO_2, SO_2, and NH_3) and other typical molecules present in the atmosphere (H_2O, N_2 and O_2), we have found the potential use of MBenes not only as gas sensors but also as gas capturers with the consequent possibility of gas removal.

The four publications included in this dissertation form a coherent set of studies on two-dimensional boron-based materials and their interactions with small molecules, highlighting the impact of adsorption on the physicochemical properties of these systems.