A DFT study of the influence of hazardous molecules on MBenes

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Abstract

The increasing amount of greenhouse gases like CO_2 and toxic gases like NO_2, SO_2, and CO due to the massive industry and engine exhaust are putting in danger the environment and climate evolution, also influencing negatively the quality of people. 2D materials are in the focus due to their high surface-to- volume ratio and stability, and can be useful for gas sensing, chemical adsorp- tion, and catalytic proposals. Among all of them, we have chosen MBenes due to their excellent electronic, thermal, transport, mechanical, and physico-chemical properties. In addition, MBenes exhibit a great capability of adsorption of small molecules, which could lead to their application in gas sensing, gas capture, and catalysis. Another advantage of MBenes is that they do not need surface passi- vation for stabilization. As newcomers to the family of 2D materials their research is still mostly lim- ited to theoretical investigations, although some of them have already been ob- tained experimentally. The stability and properties of Cr/Fe/Zr-based MBenes was presented in our previous works [1, 2]. In this work, we perform first- principles calculations to investigate the adsorption of eight molecules, CO, CO_2, H_2O, NH_3, NO_2, SO_2, O_2, and N_2 on Cr_2B_2, Fe_2B_2, and Zr_2B_2 (for adsorption energies see figure below). We also assess the potential of the three MBenes as catalysts, gas adsorbents, or gas sensors. The possible affinity for the water molecule, present in humid environments, is also considered. To this end, optimal adsorption sites, charge transfer, electronic structure, and magnetism is systematically investigated using different theoretical approaches to understand the mechanisms that govern the interaction between the gas molecules and the MBenes.

References

[1] Isabel M. Arias-Camacho. "Influence of the Hubbard U Parameter on the Structural, Electronic, Magnetic, and Transport Properties of Cr/Fe/Zr- Based MBenes". In: ACS Omega 8.47 (2023), pp. 45003–45012.

[2] Isabel M. Arias-Camacho and Nevill Gonzalez Szwacki. "Exploring the Structural, Electronic, Magnetic, and Transport Properties of 2D Cr, Fe, and Zr Monoborides". In: Materials 16.14 (2023).

Figures

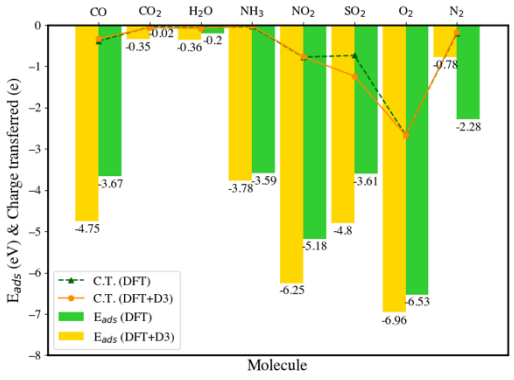

Figure 1: Adsorption energies (in eV) and charge transfer towards the molecule (in e) for molecules on orthorrhombic Cr_2B_2 MBene.