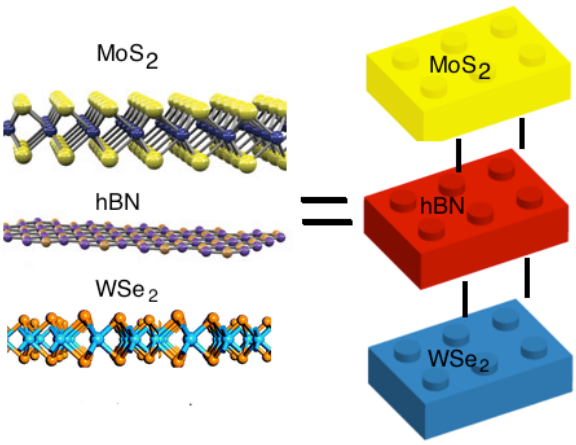

DESCRIPTION FOR THE GENERAL PUBLIC (IN ENGLISH)

Theoretical study of structural, electronic, magnetic, and optical properties of the van der Waals heterostructures containing 2D materials.

You may have heard of graphene, representative of two-dimensional materials (2D), exhibiting extraordinary properties. Nowadays, there are plenty of 2D structures available like hBN, MoS_2 under extensive research investigations. These, and other materials yet to be discovered will be used, like Lego pieces to build van der Waals heterostructures. By stacking multiple 2D structures in different configurations, one can take advantage of different properties in each of them, as well as own unique properties exhibiting by the heterostructure itself. Nowadays, only few heterostructures have been synthetized. Moreover, systematic experimental studies of potentially interesting heterostructures are impracticable (each of the heterostructures needs different synthesis method). In this regard, the high-throughput calculations will be performed in order to point out the best candidates for desirable electronic, magnetic, and optical properties. Moreover, our studies will provide reach understanding of the physical mechanisms that govern the vdW heterostructures, and therefore, to facilitate the new generation of smaller, faster, more environmentally friendly, and cheaper devices. The only theoretical tool that could guarantee the reliable prediction of the properties of vdW heterostructures is a Density Fucional Theory, in the realization of the Kohn-Sham formalism, with the weak van der Waals forces included. Those forces are of crucial importance for a correct description of the studied materials, and the approach to include them goes beyond the standard approximations used in DFT calculations. From that point of view the project describes novel scientific research that goes beyond the standard calculations of material science.