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New two dimensional compounds: beyond graphene

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In the field of nanosciences, the quest for materials with reduced dimensionality is only at its beginning. While a lot of effort has been put initially on graphene, the focus has been extended in the last past years to functionalized graphene, boron nitride, silicene, and transition metal dichalcogenides in the form of single layers. Although these two-dimensional compounds offer a larger range of properties than graphene, there is a constant need for new materials presenting equivalent or superior performances to the ones already known. Here I will present an approach that we have used to discover potential new two-dimensional materials. This approach corresponds to perform datamining in the Inorganic Crystal Structure Database using simple geometrical criterias, and allowed us to identify nearly 40 new materials that could be exfoliated into two-dimensional sheets. Then, their electronic structure (density of states and bandstructure) was obtained with density functional theory to predict whether the two-dimensional material is metallic or insulating, as well as if it undergoes magnetic ordering at low temperatures. If time allows, I will also present some of our recent results concerning the electronic structure of transition metal dichalcogenides bilayers.