

Abstract Submitted
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Interaction of water molecules with hexagonal 2D systems. A DFT study¹ NGELA ROJAS, RAFAEL REY, Universidad Nacional de Colombia — Over the years water sources have been contaminated with many chemical agents, becoming issues that affect health of the world population. The advances of the nanoscience and nanotechnology in the development new materials constitute an alternative for design molecular filters with great efficiencies and low cost for water treatment and purification. In the nanoscale, the process of filtration or separation of inorganic and organic pollutants from water requires to study interactions of these atoms or molecules with different nano-materials. Specifically, it is necessary to understand the role of these interactions in physical and chemical properties of the nano-materials. In this work, the main interest is to do a theoretical study of interaction between water molecules and 2D graphene-like systems, such as silicene (h-Si) or germanene (h-Ge). Using Density Functional Theory we calculate total energy curves as function of separation between of water molecules and 2D systems. Different spatial configurations of water molecules relative to 2D systems are considered. Structural relaxation effects and changes of electronic charge density also are reported.

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