MoS_2 decoration study. Origin of strong binding and inertness

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Nowadays the some of the most developing areas of investigations of two dimensional materials are the investigations of graphene and MoS_2. Graphene is semimetall with zero band gap displays amazing electronic, mechanical and optical properties. MoS_2 belongs to the family of transition metal dichalcogenides with semiconductor bulk band gap about 1.6 eV depending of the thickness. Graphene and MoS_2 have a complementary physical properties. So it is natural to investigate possible ways to combine these materials to create heterostructures.

Set of numbers of the layers of various compounds allows to create heterostructures by combining the layers between each other. Only the drawback of obtained heterostructure is the weak van der Waals interaction between the layers. To improve a weak interaction an individual metal atoms could be adsorbed on the layers surface before the creation of the hererostructure.

In this work detailed investigation of decoration process of MoS_2 layer by Mo atoms was performed. Using DFT calculations adsorption barrier was calculated. It was found the string binding between the MoS_2 layer and Mo adatoms which states about energy favorability of adsorption process. Further detailed investigation of the step by step decoration process and migration barrier of adatom on the MoS_2 surface to understand the origin of strong binding with taking into account inertness nature of MoS2 layer was carried out. Electronic properties were also studied during the decoration process.

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