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The effects of impurities on the structural and electronic properties[1] NATALIA CORTÉS, LUIS ROSALES, PEDRO ORELLANA, Universidad Técnica Federico Santa María, ANDRÉS AYUELA, JHON GONZÁLEZ, Material Physics Center and Donostia International Physics Center — In this work we explore the effects of molybdenum (Mo) and sulfur (S) atoms placed in two differents positions in the interlayer region of MoS_2 bilayer. By means density functional theory (DFT) calculations we have determinated that these impurity-atoms can be adsorbed in the interlayer region. Structurally, this impurity atoms causes the interlayer repultion and therefore separate the layers, decoupling the bond and breacking the equilibrium position between them. This could be used to exfoliate MoS_2 layers. Adittionaly, we found that the adatoms produce impurity states in the band gap region of MoS_2 pristine bilayer. The configurations with S impurities are semiconductors without spin polarization, whereas, when Mo impurities are located within the interlayer region, produce total spin polarization at the Fermi level.

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