Bilayered MoS2/graphene structures with a Re-atom in a supercell: theoretical studies of stable geometries and electronic properties

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Last time quasi-two-dimensional transition metal dichalcogenides Mo(W)S2(Se2) are taking attention by their semiconducting properties in contrast to semimetallic graphene ones, that they have advantage of their using in semiconductor electronics [1]. At the same time multi-layer structures [2] including bilayers of Mo(W)S2 and graphene (G) are of interest by possibilities of controlling of the electronic and electro-optic properties.

We propose new energetically stable MoS2/G90o form of bi-layers with 90o rotated graphene (G) regarding MoS2 layer, and consider by DFT simulations Mo(Re)S2/G structures with renium atom as a doping one in MoS2 supercell, or as an embedded atom between these two layers – MoS2/(Re)/G structures. Insertion of Re atoms into the MoS2-graphene structures determines their metallic properties, especially in MoS2/(Re)/G90o structure (Fig.) with high electronic density of states near Fermi level unlike semi-metallic graphene and Mo(Re)S2/G bilayer [3]. These structures may be important for the application as good metal nanoelements in electronics.

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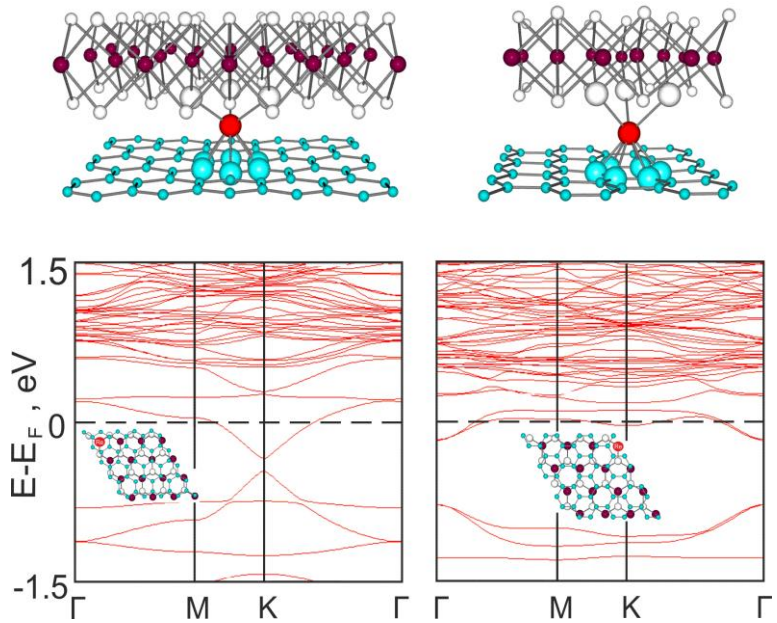

Fig. Structures with the rhenium atom between MoS2 and G layers: a common view of MoS2/(Re)/G modification(a) and bellow the band energy structure with unit cell in inset (EF= -3.52 eV), the similar schemes of the MoS2/(Re)/G90o bilayer - (b), (EF= -3.38 eV).