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Iron- and Silicon-Intercalated Graphene on Silicon Carbide: from Hybridization to Quasi-Freestanding Bilayer Graphene

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Abstract. The intercalation approach has been used for the synthesis of the ultrathin films of iron and its silicides under graphene grown on silicon carbide. Experiments have been carried out under ultrahigh vacuum conditions. The use of low energy electron diffraction together with photoelectron spectroscopy allowed to trace chemical state, elemental composition, and structural changes of the samples at all stages of synthesis. The optimal conditions of iron and silicon intercalation are realized in the temperature range of 400-500 ºC. Subsequent intercalation of graphene with Fe and Si leads to the formation of Fe-Si solid solution layer covered with Fe_3Si surface silicide. First-principles calculations were carried out using density functional theory. It is shown that iron silicide formation is accompanied by the relaxation of the buffer layer and its transformation to the second layer of graphene.

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