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**First-principles study of hybrid Graphene/MnO<sub>2</sub> bilayers**

MIGUEL PRUNEDA, Centro de Investigación en Nanociencia y Nanotecnología (CIN2-CSIC) — Oxide nanosheets are an important and promising component for creating new materials. Their capacitance properties are particularly appealing for electric batteries. Manganese oxide nanosheets are abundant, environmental friendly, have low cost, and high electrochemical activity. However MnO<sub>2</sub> poor electrical conductivity and chemical stability limits its applicability as electrode material. Hybrid graphene/oxide nanostructures have been proposed to overcome these difficulties. Here, density functional theory calculations are performed to better understand the electronic properties of heterobilayers made from graphene and MnO<sub>x</sub> monolayers. The charge transfer between graphene and MnO<sub>2</sub> monolayers are analyzed and related to the presence of oxygen vacancies in different concentrations, which are known to induce atomic reconstructions and phase transformations of the oxide. Magnetic properties of the heterobilayers will also be discussed.

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