

Abstract Submitted
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Manipulating individual defects in graphene/BN heterostructures: a first-principles study LEDE XIAN, ANGEL RUBIO, Univ of the Basque Country — Recent experiments have demonstrated the possibility of manipulating defects in insulating hexagonal boron nitride (hBN) within a graphene/hBN heterostructure using scanning tunneling microscopy, opening a new pathway of manipulating individual defects of insulators at the nanoscopic scale. With first principle calculations, we are able to simulate this process and elucidate the relevant physics in experiments. Moreover, we calculate the band level alignments between graphene and possible defects states in hBN. Thus, we identify different defects observed in experiments and provide important reference for future experiments and applications.

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