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Van der waals heterostructure of phosphorene and graphene: Tuning the Shottky barrier and doping by electrostatic gating[1]

JOSE EDUARDO PADILHA DE SOUSA, ADALBERTO FAZZIO, Universidade de Sao Paulo, ANTONIO JOSE ROQUE DA SILVA, Universidade de Sao Paulo/Laboratorio Nacional de Luz Sincrotron — Van der Waals heterostructures of 2D materials is one of the most promising approaches in terms of the new nanodevices. One of these 2D materials that have attracted a lot of attention from a broad community is the phosphorene, an elemental material composed only of phosphorus. If one wishes to build devices, two important points must always be addressed: how to make contacts - and the value of the resulting Schottky Barrier Height (SBH) - and how to control the charge doping level. In the present work we study the structural and electronic properties of single and bilayer phosphorene with graphene. We show that both the properties of graphene and phosphorene are preserved upon its contact. We also show that via the application of a perpendicular electric field it is possible to tune the position of the band structure of phosphorene with respect to that of graphene. This leads to a great control of the Schottky barrier height and doping of phosphorene, which are important features in the design of new devices based on this kind of structure.

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