Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Two-dimensional van der Waals p-n junction of InSe/Phosphorene JOSE EDUARDO PADILHA, Universidade Federal do Paran Jandaia do Sul, ROBERTO HIROKI MIWA, Universidade Federal de Uberlandia, ANTONIO JOSE ROQUE DA SILVA, Laboratorio Nacional de Luz Sincrotron, ADALBERTO FAZZIO, Universidade Federal do ABC — We investigate the energetic stability, the structural and electronic properties of van der Waals heterostructures composed by a combination of single layer InSe, bilayer phosphorene (BP), and graphene. We found that a single layer of InSe stacked on graphene (InSe@G) present a n-type Schottky barrier, which can be tuned by applying an external electric field perpendicularly to the InSe/G interface ($E_{\perp}^{\text{ext}}$). Upon further increase of $E_{\perp}^{\text{ext}}$ we may promote a n-type doping of the InSe layer. This is in contrast with the other semiconductor/metal vdW heterojunction, BP@G, where the BP sheet becomes p-type doped as a function of $E_{\perp}^{\text{ext}}$. By considering a semiconductor/semiconductor vdW system, namely BP@InSe, we found that lowest (highest) unoccupied (occupied) states lie on the InSe (BP) layers. The BP/InSe interface presents a type-II band alignment. Exploiting the electron-hole separation in BP@InSe, and the formation of ohmic contacts in InSe@G and BP@G, tuned by $E_{\perp}^{\text{ext}}$, we propose a p-n junction composed by p-type BP and n-type InSe, with the graphene acting as electrodes and also as a source of electrons/holes in the n-type/p-type InSe/BP heterostructure.

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Date submitted: 08 Nov 2016 Electronic form version 1.4