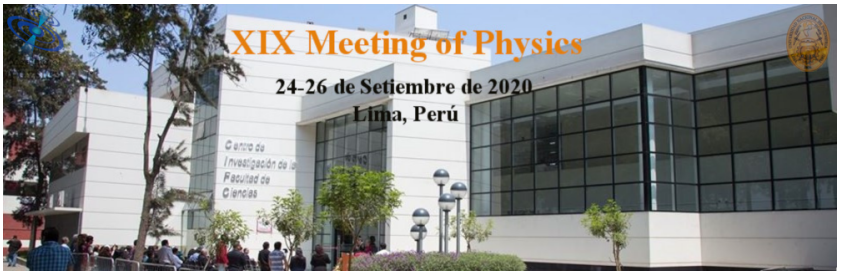

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Optical properties of atomically thin semiconductors: The role of excitons

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Two-dimensional (2D) atom-thick crystals such as graphene, boron-nitrade (BN), transition metal dichalcogenides (TMDC) and most recently phosphorus allotropes have drawn both experimental and theoretical interest due to their unique electronic and optical properties. For instance, TMDCs possess remarkable properties concerning the tunability of band gap and strong light-matter coupling that are desirable features for optoelectronic applications. Likewise, the phosphorus allotropes (black and blue phosphorus) possess layered-tunable band-gap properties and a peculiar anisotropic crystalline structure, which are important features that can be used in photonics and photovoltaics technologies.
Motivated by this recent findings and considering the individual properties of the materials mentioned above, we carry out density functional theory (DFT) calculations combining with the GW-Bethe-Salpeter (GW-BSE) methodology to study the excitonic, optical properties and the power conversion efficiency of $MoTe_2$/InN heterostructures. First, we study the geometric and electronic structure of six heterostructures based on different stacking. We also explore the effects of the tensile strain on engineering the bandgap of the individual monolayers. Secondly, we use the GW-BSE methodology to study the optical spectrum and estimate the power conversion efficiency of the device. Our results indicates that the optical band gap of the heterostructures are in the range of 1.12 to 1.17 eV [1]. For the sake of completeness, the excitonic properties of black/blue phosphorus as a function of the light-polarization are also explored [2]. We hope this work will shed some light in the seeking of designing more efficient photovoltaics devices based on those materials.
Keywords: Black phosphorus, blue phosphorus, optical properties, excitons, $MoTe_2$

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[2] C.E.P. Villegas et. al Physical Chemistry Chemical Physics 18, 27829 (2016).

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