Dielectric properties and charge density distribution in Cs-doped Black-Phosphorus

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The high carrier mobility and layer-dependent direct bandgap of Black Phosphorus (BP), makes it an extremely interesting and promising 2D material for nanoelectronics and optoelectronic applications [1]. In electrostatically gated few-layer BP, gap-tuning over a wide energy range - from the visible up to the infrared - has been observed and attributed to a giant Stark effect [2], the electric field established across the sample affecting both the energy and the spatial localization of the conduction (CB) and valence (VB) bands. As demonstrated by Kim et al. [3], tuning the energy gap E_G is also possible by adsorbing alkali metals (i.e. K, Cs) on the BP surface. According to their model, the induced electric field is localized in the first layers below the surface, the CB being localized in the topmost one, while VB states are confined in the subsurface.

In this work, we provide a comprehensive description of the electronic and dielectric properties of Cs-doped BP by combining Ultraviolet photoelectron spectroscopy (UPS) and High-Resolution Electron Energy Loss Spectroscopy (HREELS). Besides monitoring VB downward shift and E_G reduction, UPS provides also an estimate of the CB electron density. Analysis of the HREEL spectra - based on a multilayer dielectric model [4] - allows on the other hand to determine a step-profile of the Cs-induced free-carrier density along the z axis (see Fig.1 (c)). For low doping, the quasi-elastic peak narrowing is rationalized introducing a ~ 10 nm-thick intrinsic layer - due the recombination of the bulk holes with the Cs-donated electrons - on top of the p-doped semi-infinite bulk. For higher doping, when E_G reduces to 0.1 eV, a few-layer thick n-doped surface layer must be also introduced, as shown in Fig 1, right panel. These results are discussed and compared with the charge profile obtained using the non-linear Thomas-Fermi screening model, following [5].

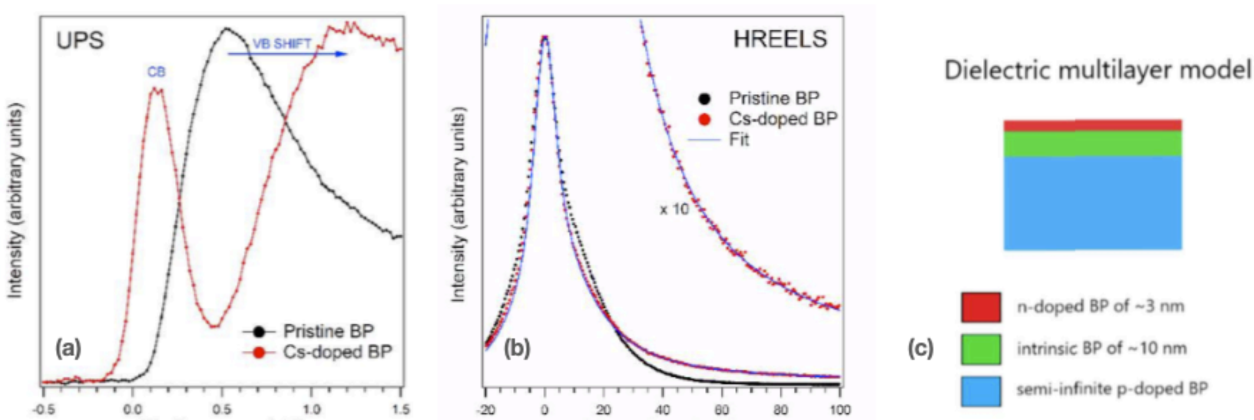

Fig. 1. (a) UPS and (b) HREELS spectra for pristine ad Cs-doped samples. (c) The dielectric model for high doping.

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