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Ab-initio study of doped bilayer graphene PAOLA GAVA, MICHELE LAZZERI, A. MARCO SAITTA, FRANCESCO MAURI, IMPMC, Paris, France — The recent discovery that the application of an external electric field induces a band gap opening in bilayer graphene [1], attracted a lot of interest on this system, due to important applications in nanoelectronics. By means of ab-initio calculations, we investigated the electronic properties of doped bilayer graphene, in presence of different bottom and top gate. In particular, the dependence of the band gap on the doping, on the average external electric field and temperature has been analysed. We find that our ab-initio results differ with respect to those obtained with standard Tigth Binding (TB) calculations [2]. In particular, we show important charge effects, which are crucial for the description of the electronic properties of bilayer graphene, and which are not included in TB models. Moreover, we compare our results with experimental measurements of the band gap, cyclotron mass and work function. [1] Ohta et al., Science v.313 , 951 (2006). [2] Castro Neto et al., Pys. Rev. Lett. v.99, 216802 (2007).

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