Electronic structure and bonding properties of potassium (K) on graphite under external electric field. ALEJANDRO TAPIA, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico., GABRIEL CANTO, Centro de Ciencias de la Materia Condensada, UNAM, Mexico. — The effect of an external electric field on the potassium (K) adsorption on the graphite surface, are studied by means of first-principles total-energy calculations. The results were obtained with the pseudopotentials LCAO method (SIESTA code) and the Generalized Gradient Approximation (GGA) for the exchange-correlation potential. The structural parameters, bonding properties, and electronic structure of the K-graphite system are studied in the triangular $(2 \times 2)$ overlayer phase as a function of the external electric field magnitude. We find an important change in the K-graphite bonding as a consequence of the charge transfer from the adatom towards the substrate induced by the electric field. The results are discussed in the light of the experimental observed diffusion of K into graphite induced by external electric fields. This work was supported by Consejo Nacional de Ciencia y Tecnología (CONACYT, México) under Grants No. 43830-F and No. 44831-F.