Electronic structure and bonding properties of K and K$^+$ on graphite under external electric field$^1$ ALEJANDRO TAPIA, ROMEO DE COSS, Department of Applied Physics, CINVESTAV-Merida, Mexico., GABRIEL CANTO, CCMC-UNAM, Ensenada, Mexico. — The effect of an external electric field on the adsorption of K and K$^+$ on the graphite (0001) 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 and K$^+$-graphite system are studied in the triangular (2x2) overlayer phase as a function of the external electric field magnitude. We find an important change in the K and K$^+$-graphite bonding as a consequence of the charge transfer from the adatom towards the substrate induced by the electric field. However, we find that none of the investigated systems show diffusion of K or K$^+$ into graphite even with a strong electric field. The results are discussed in the light of the experimental observed diffusion of K into graphite, presumably induced by external electric fields.

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