Abstract Submitted
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**Ab-initio study of hydrogen atom pairs adsorption on potassium doped graphene**[1] JORGE-ALEJANDRO TAPIA, CESAR RENAN, FI-UADY, GABRIEL CANTO, CICORR-UACAM, RUBEN MEDINA-ESQUIVEL, FI-UADY, R. DE COSS, CINVESTAV-Merida, SIMULACION DE NANOMATERIALES TEAM — The effects of the interactions of hydrogen (H) atoms on graphene (G) with potassium (K) pre-adsorbed, were predicted by means of first-principles calculations. The results were obtained with the pseudopotentials method and the generalized gradient approximation for the exchange-correlation potential. The structural parameters, bonding, electronic structure and magnetic properties of two H atoms on potassium doped graphene (2H-K/G) system are calculated by molecular dynamics. We found an important charge transfer from the K atom towards the G surface when an H atom was adsorbed, producing a chemical bonding transition from $sp^2$ to $sp^3$ in the bonded carbon atom. The binding energy per H atom was greater in the 2H-K/G system than both H-K/G and a H atom on the single G systems (H/G). The present results suggest that the hydrogen adsorption on graphene layer could be modulated by the pre-adsorption of potassium.

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