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**Simulations of noble gases adsorbed on graphene**[1] SIDI MAIGA, SILVINA GATICA, Department of Physics and Astronomy, Howard University —
We present results of Grand Canonical Monte Carlo simulations of adsorption of Kr, Ar and Xe on a suspended graphene sheet. We compute the adsorbate-adsorbate interaction by a Lennard-Jones potential. We adopt a hybrid model for the graphene-adsorbate force; in the hybrid model, the potential interaction with the nearest carbon atoms (within a distance $r_{\rm nn}$) is computed with an atomistic pair potential $U_{\rm a}$; for the atoms at r>$r_{\rm nn}$, we compute the interaction energy as a continuous integration over a carbon uniform sheet with the density of graphene. For the atomistic potential $U_{\rm a}$, we assume the anisotropic LJ potential adapted from the graphite-He interaction proposed by Cole et.al. This interaction includes the anisotropy of the C atoms on graphene, which originates in the anisotropic $\pi$-bonds. The adsorption isotherms, energy and structure of the layer are obtained and compared with experimental results. We also compare with the adsorption on graphite and carbon nanotubes.

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