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Molecular dynamics simulations of H_2O, NO_2, and N_2 mixtures on graphene.[1] HAWAZIN ALGHAMDI, SILVINA GATICA, Department of Physics and Astronomy, Howard University — In this work we study the adsorption of mixtures of H_2O, NO_2, and N_2 on graphene using the method of Molecular Dynamics. We run the simulations at constant temperatures from 100K to 230K. The H_2O and NO_2 molecules are modeled as a rigid 3-point systems and N_2 is considered a spherical super-atom with Lenard-Jones interactions. The substrate is a rigid graphene layer located at the bottom of the simulation cell. The LJ parameters of interaction between the molecules and the graphene are calculated by fitting the atomistic pair-wise sum of carbon-atom interactions with the 9-3 potential. We calculate the selectivity of NO_2/N_2 and H_2O/N_2 on graphene to test the capability of graphene to separate nitrogen dioxide or water from air.

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