

Abstract Submitted
for the MAS16 Meeting of
The American Physical Society

Adsorption of Gases on Graphene¹ HAWAZIN ALGHAMDI, SILVINA GATICA, Howard University — We simulate the adsorption of H₂O, NO₂, and N₂ on graphene using the method of Molecular Dynamics. The simulations are done at constant temperature that ranged from 100K to 250K. The H₂O and NO₂ molecules are modeled as a rigid 3-point system with Lennard-Jones and Coulomb's interactions. The motivation of the work is to test the capability of graphene to separate water or Nitrogen Dioxide from the air. We have found that a film forms on graphene at the lowest temperatures. .

¹This work is supported by the Cultural Mission of Saudi Arabia

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Date submitted: 07 Sep 2016

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