Abstract Submitted
for the CUWIP22 Meeting of
The American Physical Society

COMSOL Simulations of molecular sieve based Gas Sensor[1]
KENDRA RIVERS, Suffolk County Community College/University of Maryland, College Park, KEVIN DANIELS, University of Maryland — The gas sensing mechanisms of robust and selective solid state gas sensor, composed of electrodeposited, 2D layered manganese dioxide (MnO2) synthesized on quasi-freestanding epitaxial graphene (EG) on silicon (SiC) heterostructure is explored. The large interlayer spacing of MnO2 of 0.74 nm, can act as a molecular sieve, increasing the selectivity of the heterostructure sensor by rejecting larger molecules. The interlayer can also be tuned though intercalation of cations, which can increase the permeance of target gases. The permeance of gases, with varying kinetic diameters through these interlayers is not well understood. Using the Particle Tracing for Fluid Flow physics module in COMSOL shows the interaction of molecules within the interlayer spacing being investigated, observing the molecular sieving capabilities of the heterostructure to validate its potential as a selective gas sensor. Our results will show the 0.364nm size particles (Nitrogen) flowing towards the MnO2 layers, from here we can either see the particles are rejected or flowing through the layers which in both scenarios increases the selectivity. Additionally, we designed a built-in potential model to show electrical interaction within the MnO2-EG heterostructure with gold contacts. The simulation from the built-in model gives results of the electric potential, electron concentration and hole concentration, which shows the flow of the current with the charge potential. The results we gain from the simulation models are used to compare with physical experimental results of the gas sensor.

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Date submitted: 14 Jan 2022 Electronic form version 1.4