

Abstract Submitted
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Selectivity of adsorption of gases on doped graphene¹ JORDAN NNABUGWU, Morgan State University, SIDI MAIGA, SILVINA GATICA, Howard University — We report our results on the selectivity of carbon dioxide being adsorbed onto doped graphene. Using the Ideal Adsorption Solution theory (IAST) we calculate the selectivity using the uptake pressures of pure gases. We focus on the adsorption of atmospheric gases such as carbon dioxide (CO₂), Nitrogen (N₂), and Methane (CH₄) on a pure and doped monolayer graphene slab placed at the bottom of a simulation cell. Grand Canonical Monte Carlo (GCMC) simulations allow us to calculate the amount of gases adsorbed at a given temperature and pressure of the system. We found that including impurities of varying strength and concentration can increase significantly the selectivity at room temperature.

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