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Simulation of Adsorption of Carbon Dioxide and Methane on Graphene Sheet.[1] SIDI MAIGA, Student, SILVINA GATICA[2], None — Carbon dioxide (CO2) and Methane (CH4) constitute 90% of the annual greenhouse emission. These gases are emitted from multitude of sources such as: power station, transportation fuels, industrial processes, and agricultural byproducts. Scientists around the globe are looking for materials capable of capturing, separating, and storing these gases. Graphene with its high specific surface area provides a great platform for gas adsorption and separation. Adsorption is defined as the attachment of atoms, or molecules of a gas, liquid or dissolved solid onto a surface, creating a film or monolayer of material onto the adsorbing surface. Using the Method of Grand Canonical Monte Carlo, we computed the adsorption of carbon dioxide (CO2) and methane (CH4) on a monolayer graphene sheet, at various temperatures for each gas. For each temperature, we compute the adsorption isotherm, Energy gas-surface and Energy gas-gas. We compare the uptake pressures of CO2 and CH4. Using the Ideal Adsorbed Solution Theory (IAST), we predict the selectivity of a mixture CO2/CH4.

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