

Abstract Submitted
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Physical Adsorption of noble gases on a monolayer graphene sheet using Grand Canonical Monte Carlo Simulation¹ SIDI MAIGA, Student, SILVINA GATICA, Howard University — 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 Ar, Kr, and Xe 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, radial distribution function and structure function. We constructed the phase diagrams for 2D Ar and Kr on graphene.

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