



## Surface adsorption of carbon monoxide and hydrogen gases mixed with boron nitride (7 ,7) nanotubes by Monte Carlo method

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### Abstract

In this project, the pure adsorption of mixtures of hydrogen and carbon monoxide on nanotubes (7 and 7) of boronitrile nanotubes was studied by Montecarlo method. The potential for the interactions of gases with each other and with a nanotube according to the Lennard-Jones equation and its parameters are calculated according to Lawrence-Bartwell rules for interaction between gas, gas and gas-nanotubes. Simulation of adsorption of gases at different temperatures and pressures and the results of gas adsorption density are calculated and compared in each case. The results show that the adsorption of gases is directly related to the increase of pressure and with the increase of temperature, the relation is opposite. Comparison of the results shows that absorption is higher in pure state.

**Keywords:** Surface adsorption, single-wall nano-tubes of boron nitride, Monte Carlo simulation, density, carbon monoxide gas and hydrogen

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### 1. Introduction

Today's world is the era of substructures and our goal is to achieve self-sufficiency and independence in this area. Technology, technology, and nanotechnology. The first nano spark during a Fayman lecture, with the statement that "there is a lot of space at a low level" was introduced for nanotechnology. He It has been suggested that individual atoms can be manipulated and produce small materials and structures that have different properties [1]. So, after nearly a year, today, it has achieved