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MOLECULAR DYNAMICS STUDY OF METHANE AND HYDROGEN SULPHIDE IN Li^+ DOPED SINGLE WALL CARBON NANOTUBE.

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Abstract. On this work, was performed the isothermal curves of methane and hydrogen sulphide adsorption in a single wall carbon nanotube (CNT) doped with five lithium ions. The results have shown the major adsorption of H_2S than methane molecules. However, these same results are strongly dependents of the temperature. For the same molecular concentration, the increasing of temperature decreases the number of adsorbed molecules.

The massive presence of acid gases, thus like carbon dioxide and hydrogen sulphide are hard problem on many oil and gas reserves. On this work, the adsorption process was employed to study the removal of hydrogen sulphide from its equimolar mixture with methane. The carbon nanotubes are pointed a promissory material for adsorption because of its specific area [1]. Today this technology is already used on molecular sieves and to gas storage. The lithium ions are kept frozen narrow CNT at distance of a typical carbon-lithium bond. Lennard-Jones 12-6 coupled with the Coulomb electrostatic potential were used to simulate the intermolecular interactions. The simulated CNT was a single wall armchair carbon nanotube, with 208 carbon atoms, 26.09 Å of length and 3.08 Å of radius. Five lithium ions (Li^+) were randomly fixed at the carbon-lithium at 1.494 Å [10]. Both methane and hydrogen sulphide molecules are kept frozen during the simulation. Figure 1 shows the final configuration of simulated box, where: sulfur atom is yellow and carbon atom is green. Figure 2 shows the radial distribution function between the CNT carbon and the H_2S with temperature. Since the curves have the same pattern one can conclude that the type of interaction between the CNT and H_2S molecules is not changed by the temperatures action. However, as the intensity of the curves increases with temperature, the number of adsorbed molecules decreases with temperature increasing. The behavior of number of adsorbed molecules with the temperature is showed in a Figure 3.

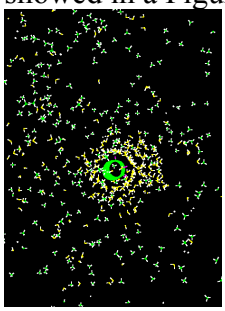

Figure 1. Final configuration.

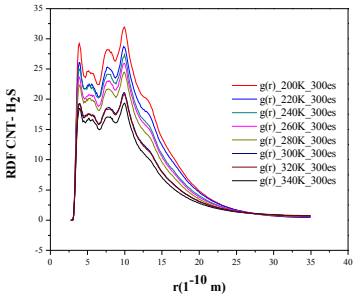

Figure 2. Temperature effect on RDF curve

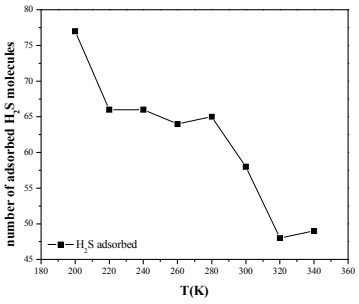

Figure 3. Temperature effect on adsorbed number.

References.

[1] Dresselhaus, M. S., Dresselhaus, G. e Avouris, Ph., "Carbon Nanotubes: Synthesis, Structure, Properties and Applications", 1ed, Springer Press, 2001.

[10] Borodin, O., Smith, G. D., and Fan, P. "Molecular Dynamics Simulations of Lithium Alkyl Carbonates", J. Phys. Chem. B 2006, 110, 22773-22779.