Sensor using molecular dynamics of natural gas in carbon nanotubes under the external uniform electric field

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Abstract

Natural gas (NG) is a naturally occurring gas mixture that is formed under the surface of the Earth. (NG) is considered the cleanest fossil fuel and is a safe source of energy when transported, stored and used[1]. Due to the various limitations of techniques currently available for detection of (NG) the research on new detection systems is still thriving [2], one of them being the use of carbon nanotubes (CNTs). We can with the help of molecular dynamics (MD) make a theoretical study on the physico-chemical properties of (NG) (EOT), in situ temperature, molar entropy variation (ΔS) and the distance between the center of mass of the molecule and the carbon nanotube Armchair (9,9) [3] at a temperature of 1 mK of different types of molecules constituting the (NG) as (CH_4, C_2H_6, C_3H_8, C_4H_{10}, $(CH_3)_2CHCH_3$,N_2 and CO_2). The evanescent effect generated by the wall of the carbon nanotube when applied parallel and uniform electric field causes the molecules to rotate around the nanotube at high speed. It can be seen, therefore, that the system performance works like a good (NG) sensor.

Keywords: Natural Gas; Molecular Dynamics, Carbon Nanotube, Electric Field, Evanescence Effect

References

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