Optimization of hydrogen storage capacity by physical adsorption on open-ended single-walled carbon nanotube as diameter function

Nasruddin, author

Abstrak

In this paper, we perform combination methods of semi-empirical research, a theoretical approach, and force-matching to determine the optimum adsorption capacity on an open-ended single-walled carbon nanotube (SWCNT) as a diameter function. Using a semi-empirical study, we can determine the value of monolayer coverage and isosteric heat of adsorption from available thermodynamic data. By completing the semi-empirical study, we carried out quantum mechanical calculations to determine the adsorption energy on the interior and exterior of SWCNTs. Furthermore, monolayer coverage, specific surface area, and maximum adsorption capacity as the main quantity in the adsorption process was estimated using the combination method of force-matching and a classical Lennard-Jones potential model. Hydrogen physisorption was investigated on zig-zag SWCNTs at conditions for a pressure range of 0.1 to 10 MPa at 233 K and 298.15 K temperature. The adsorption of all data can be explained with the Toth model. The results shows the SWCNT exterior physisorption energy range between 1.35 to 1.62 kcal/mol. The interior range from 1.22 to 2.43 kcal/mol. With a wide degree of temperature and pressure variations, we obtained an optimum SWCNT diameter of 8-12 Å . At the optimum diameter maximum adsorption capacity, we achieved 1.75 wt% at 233 K and an operating pressure of 10 MPa.