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Comparison of doped combination zirconium-tungsten, zirconium-molybdenum and molybdenum-tungsten on single-wall vanadium oxide nanotube in hydrogen gas adsorption

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Abstract

In this study, doped vanadium oxide nanotubes were evaluated using different software to study the absorption of hydrogen gas. Vanadium oxide nanotubes are one of the options for absorption and storage hydrogen gas. In this research study for the first time, the Monte Carlo simulation was used to investigate the hydrogen gas absorption behavior in molybdenum-tungsten, molybdenum-zirconium and zirconium-tungsten doped vanadium oxide nanotub. At 300 K and at different pressures, the amount of hydrogen gas absorption inside and outside the doped nanotubes has been investigated. The results show the maximum adsorption capacity in 50MPa. Also, by comparing the obtained data and absorption isotherms, was determined absorption of hydrogen gas in vanadium oxide nanotube doped with zirconium molybdenum was better than the other two nanotubes.

Keywords: Simulation Monte Carlo (MC), Vanadium oxide nanotube (VONT), absorb,