

Abstract Submitted
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Temperature and Pressure Dependence of Hydrogen Coverage on Single-Walled Carbon Nanotubes¹ JUN NI, XIAOBAO YANG, Department of Physics, Tsinghua University — The safe and compact storage of hydrogen is of great interest in theoretical and experimental research. Carbon nanotubes are reported to be highly efficient for gas and alkali atom storage. The process of hydrogen adsorption on the carbon nanotubes is changed under various circumstances. It is important to know how the hydrogen coverage depends on the tube diameters, temperature and pressure. We have investigated the stability of various hydrogenated single-walled carbon nanotubes. We find the storage capacity of hydrogen depends significantly on the diameters of carbon nanotubes. The full hydrogen coverage can be reached for the nanotubes with small size, while for the nanotubes with large size, the saturation coverage is lower than 1. We have calculated the variation of the hydrogen coverage with the change of temperature and pressure. In particular, we find that the nanotubes with diameters of about 1 nm can achieve the coverage of 80% at ambient temperature and low pressure, which is in agreement with the experimental results.

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