Supplementary Material

Effect of Diameter

We studied the effect of diameter on hydrogen storage at a low temperature (80 K) and at roomtemperature (298 K). We found that at the low temperature as the diameter increases from ≈13 Å, storage capacity decreases, due to decrease in curvature effect, see Fig. S1. At room temperature due to increased thermal motion of the hydrogen gas molecules the van der Waals interaction decreases and the curvature effect doesn't significantly affect the hydrogen storage and hence, the gravimetric capacity remains almost constant. However, at a diameter below 10 Å, adsorption inside the nanotube becomes very difficult as shown in the density profiles (see inset plot of Fig. S2 a). For the nanotubes with larger diameter, ≈31 Å, bulk density inside the nanotube has been reached, see Fig. S2 c. Therefore, a large diameter is also not required to achieve an increased inside adsorption. Moreover, the decrease in curvature effect may decrease the storage capacity. We found that ≈13 Å diameter is an optimum one for hydrogen adsorption.

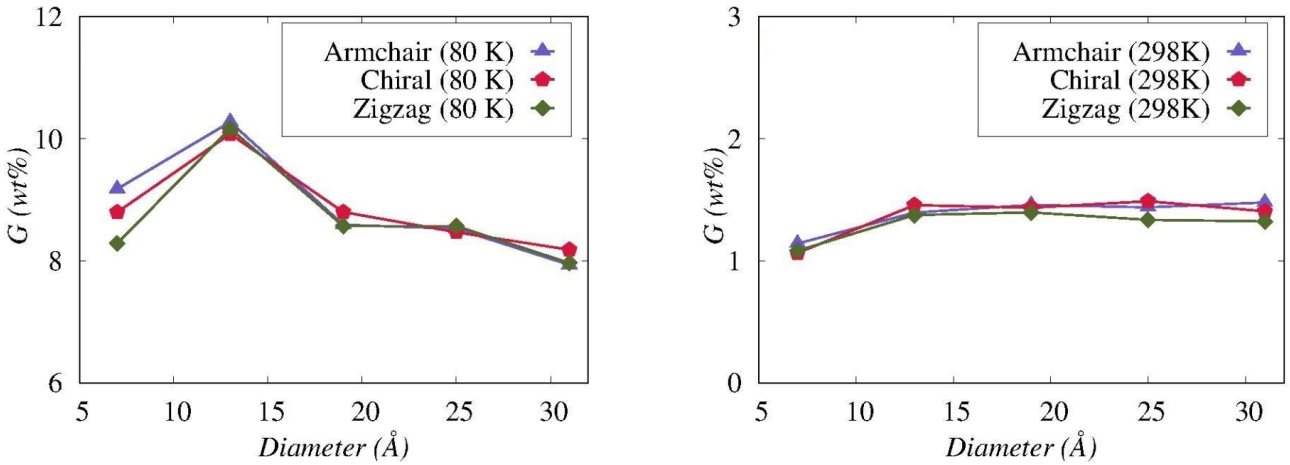

Fig. S1. (Color online) Gravimetric hydrogen adsorption for armchair, chiral and zigzag SWCNT as a function of diameter at 80 K (a) and 298 K (b).

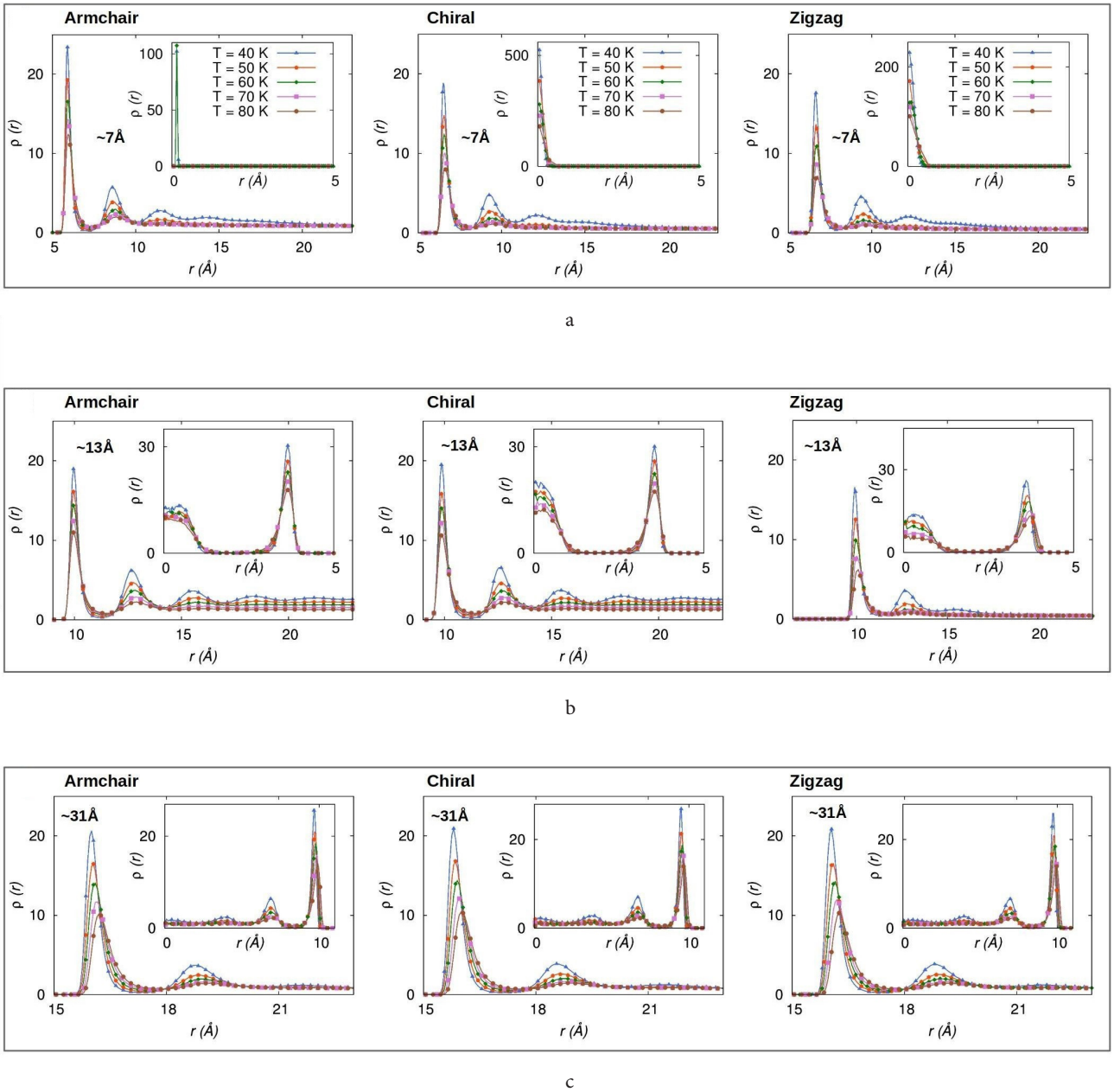

Fig. S2. (Color online) Density profile of hydrogen molecules perpendicular to the major axis of SWCNT for different diameter ≈7 Å (a), ≈13 Å (b) and ≈31 Å (c). The inset plots are the density profiles inside the nanotube and the main plots are the density profiles outside the nanotube.