

## Density Functional Study of Hydrogen Adsorption at Low Temperatures

C. Gu, G.-H. Gao<sup>C, S</sup> and Y.-X. Yu

*Department of Chemical Engineering, Tsinghua University, Beijing, P.R. China*

Because of its small size, hydrogen differentiates itself from other classical fluids with strong quantum effects at low temperatures. Classical thermodynamic treatments become inadequate in this circumstance. In the present work, as proposed first by Wigner and Kirkwood, quantum correction is introduced in the calculation of Helmholtz free energy by its Taylor expansion in powers of thermal wavelength. This quantum-mechanical free energy is used in density functional theory (DFT) to calculate the density distribution of hydrogen in single-walled carbon nanotubes. The adsorption isotherms of different tube sizes and temperatures are studied and discussed as well. In DFT, Weeks-Chandler-Andersen (WCA) is used to build the attractive contribution, and Tarazona's smoothed-density approach (SDA) is applied to make the nonlocal correlation. Path integral grand canonical Monte Carlo (PI-GCMC) simulation is also performed to test the validity of the quantum corrected density functional theory. Reasonable agreement between the results of the two methods is obtained at low bulk densities. However, when the bulk density is high, the DFT predicts too high pore densities compared with PI-GCMC results. This indicates that the present quantum correction is still inadequate in system with strong quantum effect.