Density functional theory (DFT) studies on adsorption of several gaseous homo- and hetero-diatomic molecules (AB) including H₂, O₂, N₂, NO and CO on external surface of H-capped pristine armchair (5, 5) single-walled carbon nanotube (SWCNT) were conducted. Structures of C₇₀H₁₀ and the corresponding C₇₀H₁₀–AB adducts were fully optimized at the B3LYP/6-311G* level of theory. Calculated ¹³C NMR chemical shifts were analyzed and critically compared with available experimental data. Significant changes of carbon NMR atom chemical shifts (up to –100 ppm) and shielding anisotropies (up to -180 ppm) at sites of addition were observed.

Fig. 1. The B3LYP/6-31G* optimized model of armchair (5, 5) SWCNT. A1 and A2 adsorption sites including C3, C4 and C22, C31 carbons are marked in blue. Two types of C–C bonds, tilted and perpendicular are marked off, too.