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Theoretical study of carbon-nanotube-based molecular sensors YAN LI, MIROSLAV HODAK, JERRY BERNHOLC, North Carolina State University, CENTER OF HIGH PERFORMANCE SIMULATION AND DEPARTMENT OF PHYSICS TEAM — Carbon Nanotubes (CNTs) are highly promising for chemical and biological sensing applications, owing to their high chemical and mechanical stabilities, high surface areas as well as unique electronic properties. We report results of theoretical studies of detection abilities of several small analyte molecules, such as ammonia and nitrogen dioxide. We use density functional theory (DFT) and Keldysh non-equilibrium Green's function (NEGF) formalism to investigate differences in transmission coefficients and current due to interactions between the CNT and analyte molecules. For nitrogen dioxide, which chemisorbs on the CNT, we show that its attachment produces significant differences in both transmission and Current-Voltage (I-V) curve. For ammonia, we find that it can be either physisorbed or chemisorbed on the CNT depending on its position relative to the metalic leads. The chemisorbed case shows detectable differences in transmission and I-V curve. We also investigate sensing mechanisms of CNTs functionalized with receptor molecules for specific analyte molecules.

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