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Selective sensing of ethylene and glucose using carbon-nanotube-based sensors: An ab initio investigation YAN LI, MIROSLAV HODAK, WENCHANG LU, JERRY BERNHOLC, North Carolina State University — Functionalized carbon nanotubes have great potential for nanoscale sensing applications, yet many aspects of their sensing mechanisms are not understood. We investigate two paradigmatic sensor configurations for detection of biologically important molecules through ab initio calculations: a non-covalently functionalized nanotube for glucose detection and a covalently functionalized nanotube for ethylene detection. Despite of their structural and chemical simplicities, glucose and ethylene control key life processes of humans and plants, respectively. We evaluate the sensors' electrical conductance and transmission coefficients at the full density-functional theory level via the non-equilibrium Green's function method. A clear atomistic picture emerges about the mechanisms involved in glucose and ethylene sensing. While functionalized semiconducting nanotubes exhibit good sensitivities in both cases, the current through metallic nanotubes is only weakly affected by analyte attachment. We also investigate the effects of band gaps of the nanotubes and changes to the receptors on the detection sensitivities. These quantitative results can guide the design of improved sensors.

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