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Adsorption of polar molecules on carbon nanotubes in transverse electric fields Ş.C. BĂDESCU, T.L. REINECKE, E.S. SNOW, F.K. PERKINS, V.M. BERMUDEZ, NRL, Washington DC — Experiments in our laboratory show that capacitance measurements can be used for chemical sensing with arrays of single-wall carbon nanotubes (NTs). Molecular adsorption on NTs is affected by electrostatic gating that creates intense surface electric fields. The a.c. capacitance amplitude is found to be related to the intrinsic adsorbate dipole moment. To understand the details of the processes involved, *ab-initio* calculations of molecular adsorption on graphene and on NTs with electric fields normal to the surfaces have been made. We study the dependence of adsorption energy, adsorption-induced polarizability and charge transfer on the field intensity and direction in the range 10^4-10^6 V/cm. We identify three groups of adsorbed molecules: (1) those with the dipole moment normal to the NT for which the observed capacitance depends $\sim$ linearly on dipole moment (e.g. C_3H_6O, CH_3Cl, NH_3, DMMP, CNH); (2) those with dipole moments parallel to the NT and that have little effect on the capacitance (e.g. C_6H_5Cl, $C_6H_4Cl_2$); (3) non-polar molecules (e.g. CH_4), polarized by the intense electric fields and by adsorption. The adsorption-induced dipole moment plays an important role in the total polarization. The results are consistent with the experiment, in particular with infrared spectroscopy data.

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