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Adsorption of Alcohols and Alkanes on Single-Walled Carbon Nanotubes ERIK ALLDREDGE, STEFAN BADESCU, THOMAS REINECKE, NAVDEEP BAJWA, F. KEITH PERKINS, ERIC SNOW, Naval Research Laboratory — Recent experiments with arrays of carbon nanotubes (CNTs) reveal a strong electrical response during exposure to polar alkane derivatives such as linear alcohols $C_nH_{2n+1}OH$, which is in contrast with the weak response to linear alkanes C_nH_{2n+2}. To develop an understanding of the microscopic mechanisms involved, we perform detailed *ab initio* calculations of adsorption geometries and charge configurations for the size parameter n from 1 to 8 on pristine zig-zag and armchair CNTs. We use Density Functional Theory with localized orbitals in a cluster approach, along with the M05-2X functional appropriate for the weak interactions of physisorption for these systems. We find that adsorption energies are larger for alcohols than for alkanes and increase linearly in energy with length of the molecule n for both alcohols and alkanes (at 35 meV and 40 meV per additional CH_2, respectively). This is found to be in good agreement with the binding energy per additional CH_2 estimated from the fast conductance response measurements for both alcohols and alkanes using a simple kinetic theory model. We estimate small charge transfers for all molecules, which suggest that the electric response is dominated by the scattering from the dipole moments of the adsorbates. [This work is supported by the Office of Naval Research.]

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