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Adsorption of Nitro Aromatics on Single-Walled Carbon Nanotubes ERIK ALLDREDGE, STEFAN BADESCU, THOMAS REINECKE, NAVDEEP BAJWA, F. KEITH PERKINS, ERIC SNOW, US Naval Research Laboratory — Recent experiments with arrays of carbon nanotubes reveal a strong conductivity response after exposure to aromatic molecules containing nitro functional groups, such as nitrobenzene and trinitrotoluene. The detection of these compounds is of particular interest in the use of nanotube arrays as chemical sensors. To develop an understanding of the microscopic mechanisms involved, we perform detailed *ab initio* calculations of adsorption geometries, charge configurations, and vibration spectra for these compounds on pristine armchair and zigzag nanotubes. We use density functional theory with localized orbitals in a cluster approach and the M05-2X functional that is appropriate for the weak interactions of physisorption for these systems. We find a strong increase in adsorption energy with the addition of each nitro group to a molecule (around 100 meV) and a gradual increase with nanotube size, in agreement with preliminary experimental results. For most of these compounds, little charge transfer ($< 0.1\ e$) occurs. Finally, these calculations are compared with results for the adsorption at oxidation defects.

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