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**Theoretical Investigation on Alcohol Sensing of Glycine-Coated Carbon Nanotubes**[1] TAO JIANG, UMass Lowell, GARY KUSSOW, YOUNG-KYUN KWON, Dept. of Physics, Univ. of Mass Lowell — It has been observed that single walled carbon nanotube field effect transistors (SWNT-FET) coated with glycine can be used as alcohol sensors. The original semiconducting glycine-coated SWNT-FET have been changed to be metalic in the presence of alcohol. Using *ab initio* density functional theory, we compute the structural and electronic properties of carbon nanotubes coated with glycine in the absence or in the presence of alcohol (Isopropanol) to investigate alcohol sensing mechanism. To demonstrate specificity of such glycine-coated SWNT-FETs on alcohol, we also study those properties in the presence of other molecules, such as acetone and water. Furthermore, we investigate the effect of an external fields on glycine-coated SWNT with IPA, and indentify the gate-electric-field screening in SWNT-FET to be a major role for alcohol sensing.

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