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Adsorption of 2,4,6-trinitrotoluene on the ZnO ($2\bar{1}\bar{1}0$) surface: a density functional theory study of the detection mechanism of ZnO nanowire chemiresistors[1] SUFIAN ALNEMRAT, GARY BRETT, JOSEPH HOOPER, Naval postgraduate school — We report first-principles calculations of the adsorption of 2,4,6-trinitrotoluene (TNT), a prototypical nitroaromatic explosive, on the ZnO ($2\bar{1}\bar{1}0$) surface. This surface is common among ZnO chemiresistors being considered for trace explosive detection. Recent work has achieved 60 ppb detection of TNT using a ZnO nanowire array, but the physical mechanism of sensing is unclear. Our results indicate that TNT strongly chemisorbs via interactions between the oxygen on the nitro groups and surface zinc, creating surface states within the gap. We present a simple theoretical estimate showing the strong effect of these surface states on the depletion layer of ZnO nanowires.

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