Metal-insulator transition at the interface of LaAlO$_3$/SrTiO$_3$ induced by H$_2$O adsorption  

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— We investigated the adsorption configurations at various H$_2$O coverages on the AlO$_2$ surface of n-type interface of 3 unit cell layers of LaAlO$_3$ (LAO) overlayer on SrTiO$_3$ (001) (STO) and the effects on the electronic properties at the interface by carrying out density-functional-theory calculations. For 0.25 monolayer (ML) and 0.5 ML coverages of H$_2$O the dissociation processes are barrierless. While for 1 ML coverage the mixing adsorption configuration comprising 0.5 ML molecular and 0.5 ML dissociated H$_2$O is most stable and the dissociation from fully molecular adsorption has to overcome 1 eV barrier. Insulator-metal transition at the n-type interface of (LAO)$_3$/STO occurs as the coverage of dissociated H$_2$O reaches to 0.5ML. Insulator-metal transition at the interface can be realized by two ways: (1) changing H$_2$O coverage of from less than 0.5ML to equal to 0.5ML; (2) fixing H$_2$O coverage at 1ML and converting the adsorption configuration from fully molecular adsorption to mixing (0.5:0.5) adsorption. The second scheme can be utilized to realizing single-electron controlled nanoscale memory and switch.