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Metal-insulator transition at the interface of $LaAlO_3$ /$SrTiO_3$ induced by H_2O adsorption YUN LI, School of Advanced Materials Science & Engineering, Sungkyunkwan University, Suwon, 440-746, Korea, JAEJUN YU, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, Korea — We investigated the adsorption configurations at various H_2O 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_2O 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_2O 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_2O reaches to 0.5ML. Insulator-metal transition at the interface can be realized by two ways: (1) changing H_2O coverage of from less than 0.5ML to equal to 0.5ML; (2) fixing H_2O coverage at 1ML and converting the adsorption configuration form 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.

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