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The effects of surface polarity and dangling bonds on the electronic properties of MoS2 on SiO2[1] HA-JUN SUNG, DUK-HYUN CHOE, KEE JOO CHANG, Korea Adv Inst of Sci & Tech — MoS2 has recently attracted much attention due to its intriguing physical phenomena and possible applications for the next generation electronic devices. In pristine monolayer MoS2, strong spin-orbit coupling and inversion symmetry breaking allow for an effective coupling between the spin and valley degrees of freedom, inducing valley polarization at the K valleys. However, the spin-valley coupling disappears in bilayer MoS2 because the inversion symmetry is restored. In this work, we investigate the effects of surface polarity and dangling bonds on the electronic properties of MoS2 on α-quartz SiO2 through first-principles calculations. In monolayer MoS2, a transition can take place from the direct-gap to indirect-gap semiconductor in the presence of O dangling bonds. In bilayer MoS2, O dangling bonds induce dipole fields across the interface and thus break the inversion symmetry, resulting in the valley polarization, similar to that of pristine monolayer MoS2. Based on the results, we discuss the origin of the valley polarization observed in MoS2 deposited on SiO2

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