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Band alignment study on Al/SiO_2 and Cu/SiO_2 metal-oxide interface with the presence of point defect[1] JIANQIU HUANG[2], ERIC TEA[3], CELINE HIN[4], Virginia Tech — Metal-Oxide interface has a wide use in electronic devices. Currently, technological development is aiming on the shrinkage of electronic devices' size. Based on the knowledge of electron tunneling effect, the reduction of dielectric thickness would cause an exponential increase on electron tunneling probability which contributes to current leakage. It might cause dielectric breakdown, which could make a severe and irreversible damage to the devices. Therefore, the main purpose of this study is to explore the possible factors that can lead to dielectric breakdown at metal-oxide interface. Density functional theory *ab initio* calculation has been applied to study the Al/SiO_2 and Cu/SiO_2 metal-oxide interface. Results on oxygen (di)vacancies at the interface will be presented and compared with the defect free model. The band alignment has been constructed to describe the variation of potential barrier height due to defect at interface. Results show the oxygen (di)vacancies at interface might trap electron and reduce potential barrier height. Moreover, the potential barrier height has a significant dependence on defects charge states.

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