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Band alignment study on Al/SiO_2 and Cu/SiO_2 metal-oxide interface with the presence of H atom impurity and external electric field[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 could 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. Previous study revealed the facts that oxygen (di)vacancies at interface might trap electron and vary potential barrier height. In this study, we introduced the H atom impurity at interface, and applied external electric field to the system. Charge density differences have been calculated to observe the charge alternation at the interface when impurity and external electric field existed. Band alignment revealed the potential barrier height variation due to the impurity and external electric field, which provided us how barrier height would respond to these two types of defects.

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