**Excited electron dynamics in the 1T/2H heterophase of monolayer MoS2: real-time time dependent density functional theory study for photo-catalyst application**

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Monolayer MoS2, one of the two-dimensional transition metal dichalcogenide (TMD) materials, has two different phases, 2H and 1T phases. The 2H, the stable phase, is a semiconductor with direct band gap about 2.4 eV, and 1T, the meta-stable phase, has metallic phase. The 2H phase of MoS2 has been studied and utilized as a hydrogen evolution reaction (HER) catalyst because of its photovoltaic and photo-catalytic features. On the other hand, the 1T phase of MoS2 has been investigated in the perspective of nanoscale electronic device, such as ultrathin transistor and supercapacitor electrode component. Furthermore, the heterophase boundary of 2H and 1T phases was also synthesized and its microscopic dynamics was investigated in terms of phase boundary or phase transition.

In this study, we investigated geometric and electronic structure of the MoS2 heterophase. We found that two different types of phase boundary lead to difference in the band alignments at MoS2 phase boundaries. As a consequence, the excited electrons in the 2H phase region are transferred and accumulated in the 1T phase region, leading to the charging of the 1T phase region. We performed the real-time time dependent density functional theory (rt-TDDFT) calculation for this electron dynamics. We found that, as the 1T phase is charged, the activation barrier of dissociative adsorption of oxygen molecule on the planar surface of 1T phase is decreased. In the acidic condition, the oxygen reduction reaction (ORR) energy profile on the charged 1T phase region shows similar electrochemical properties with that on the platinum (100) surface. We suggest that the MoS2 heterophase can serve as the novel low-dimensional ORR photo-catalyst.