Study on physical properties of structural elementary excitations of semiconductor surfaces and interfaces

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Our project has been focused on the physical properties of structural elementary excitations of semiconductor surface and interfaces. We have performed two topics in this year. One is the supporting effect on physical properties of vacancies of monlayer MoS_2 [1, 2]. The other is the dynamical properties of SiO_2 at the interface with Si [3, 4]. The calculations were performed based on the first-principles calculation. Program package VASP was employed.

In the first topic, we focus on the properties of vacancies of monolayer MoS_2. Our previous studies revealed that the formation energies of vacancies such as V_S, V_{S2}, and V_{Mo} are very small in case of negatively charged. We put the monolayer MoS_2 on another monolayer MoS_2, and examine the change of vacancy stabilities. The calculated results indicate that the formation energies increase by more than 0.2 eV. Further, when we put on monolayer $MoSe_2$, the formation energies increase by more than 0.5 eV. We can understand this stabilization by the vacancy stability on surfaces. Because monolayer MoS_2 is two-dimensional material and has exactly two bare surfaces, vacancies can be easily formed. However, one of the monolayer surface is covered by some other material, it is not a surface any more. Now MoS_2 has only one bare surface. Therefore, the atoms in MoS_2 interact with more atoms before, and vacancies are stabilized.

In the second topic, we focus on the oxygen vacancy effect. During oxidizing Si, we previously found that excess Si is emitted from the interface into the oxide. The excess Si in the oxide causes oxygen vacancies in the oxide. We study the effect of such oxygen vacancy on the diffusivity of Si and O in the oxide based on the first-principles molecular dynamics. We perform the study in the temperature range from 3000 K to 6000 K, and find that the incorporation of oxygen vacancy surely enhances the diffusion of Si and O. We analyze the calculated results, and successfully obtain the equation for the enhanced diffusion. When we compare the obtained equation with the empirical equation experimentally obtained previously, we find good consistencies in their activation energies, prefactors, and enhancement coefficients.

References

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