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Variation of the Si-induced Gap State by the N defect at the Si/SiO_2 Interface

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Nitrided-metal gates on the high-κ dielectric material are widely studied because of their use for sub-20nm semiconductor devices and the academic interest for the evanescent states at the Si/insulator interface. Issues in these systems with the Si substrate are the electron mobility degradation and the reliability problems caused from N defects that permeates between the Si and the SiO_2 buffer layer interface from the nitrided-gate during the gate deposition process. Previous studies proposed the N defect structures with the gap states at the Si band gap region. However, recent experimental data shows the possibility of the most stable structure without any N defect state between the bulk Si valence band maximum (VBM) and conduction band minimum (CBM).

In this talk, we present a new type of the N defect structure and the electronic structure of the proposed structure by using the first-principles calculation. We find that the pair structure of N atoms at the Si/SiO_2 interface has the lowest energy among the structures considered. In the electronic structure, the N pair changes the eigenvalue of the silicon-induced gap state (SIGS) that is spatially localized at the interface and energetically located just above the bulk VBM. With increase of the number of N defects, the SIGS gradually disappears in the bulk Si gap region, as a result, the system gap is increased by the N defect. We find that the SIGS shift with the N defect mainly originates from the change of the kinetic energy part of the eigenstate by the reduction of the SIGS modulation for the incorporated N defect.

Keywords: silicon/silica interface, N defect, first-principles

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개미산에서 수소 생산용 Pd 기반 합금 촉매의 제일원리 설계

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본 발표에서는 DFT를 사용하여 개미산으로부터 수소 생산용 Pd 기반 합금 촉매의 합리적 설계를 다룰 것이다. 특히, 합금 촉매 효과 [ligand (electronic) 및 strain effect)]가 어떻게 개미산으로부터 수소 생산의 반응성과 선택도에 영향을 미칠 수 있는지를 조사하였다. 이러한 결과는 높은 촉매 성능을 달성하기 위해서 다성분 촉매의 표면 활성을 타당하게 제어하는 것이 얼마는 중요한지를 보여준다 [J. Phys. Chem. C, 118, 22254-22560 (2014), J. Nanosci. and Nanotech., 15, 8233-8237 (2015), ACS Catalysis 6 (1), 134-142 (2016)]

Keywords: DFT, formic acid, Pd, alloy catalysts