

SW-P007

Hydroxide diffusion rates in amorphous solid water

Du Hyeong Lee, Jaehyeock Bang and Heon Kang*

Department of Chemistry, Seoul National University

We present bulk diffusion rates of hydroxide ions in amorphous solid water (ASW) at 135 ~ 160 K. Previous researches showed that the diffusion mechanism of hydroxide is different from one of hydronium ions, and this implies that they have different diffusion rates. In ultra-high vacuum (UHV) chamber, low-energy scattering (LES) was used to measure ion population and temperature-programmed desorption (TPD) was conducted for measuring ASW thicknesses. To determine the diffusion rates, a simple model for H₂O/NaOH/H₂O sandwich films was developed using Fick's second law. The measured surface population of hydroxide ions as a function of time was well fitted to the model, and the rates were well agreed to an Arrhenius equation.

Keywords: hydroxide, diffusion, amorphous solid water

SW-P008

Electronic structure of potassium-doped copper phthalocyanine studied by photoemission spectroscopy and density functional calculations

임영지, 김종훈, 지동현, 조상완

연세대학교

The metal intercalation to an organic semiconductor is of importance since the charge transfer between a metal and an organic semiconductor can induce the highly enhanced conductivity for achieving efficient organic electronic devices. In this regard, the changes of the electronic structure of copper phthalocyanine (CuPc) caused by the intercalation of potassium are studied by ultraviolet photoemission spectroscopy (UPS) and density functional theory (DFT) calculations. Potassium intercalation leads to the appearance of an intercalation-induced peak between the highest molecular occupied orbital (HOMO) and the lowest molecular unoccupied orbital (LUMO) in the valence-band spectra obtained using UPS. The DFT calculations show that the new gap state is attributed to filling the LUMO+1, unlike a common belief of filling the LUMO. However, the LUMO+1 is not conductive because the π -conjugated macrocyclic isoindole rings on the molecule do not make a contribution to the LUMO+1. This is the origin of a metal-insulator transition through heavily potassium doped CuPc.

Keywords: CuPc, PES, DFT, potassium