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Band diagram of an Alq$_3$/Nb:SrTiO$_3$ interface studied by *in situ* photoemission spectroscopy

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Introduction

Organic semiconductors (OSCs) have attracted enormous attention in the past few decades because of their potential applications to organic-based devices, such as organic light-emitting diodes. In these devices, formation of interfacial dipole layers between OSCs and metal electrodes dominates device performance, and a great number of studies have been devoted for understanding the origin of the interfacial dipole [1]. Conductive perovskite oxides are expected as candidates for electrode materials in organic devices, since they possess the advantage of high transparency and high chemical stability. However, there are few studies on the band alignment at OSC/oxide interface.

In this study, we report on the band alignment at the interface between tris(8-hydroxyquinolinato)-aluminum(III) (Alq$_3$) and conductive Nb-doped SrTiO$_3$ (Nb:STO) determined by *in situ* photoemission spectroscopy (PES) measurements.

Experimental

The Nb:STO substrate was annealed at 1050 °C and an oxygen pressure of 1×10^{-7} Torr to ensure an atomically flat TiO$_2$-teminated surface, and was subsequently annealed at 450 °C and 760 Torr to restore the surface oxygen stoichiometry. Alq$_3$ thin films with various thicknesses were deposited on the Nb:STO substrate by vacuum vapor deposition with the deposition rate of 0.1 Å/s using Knudsen cell heated at 250 °C. Subsequently, PES measurements were carried out *in situ* using MgKα (hv = 1253.6 eV) and He I (hv = 21.2 eV) with an energy resolution of 1.3 eV and 0.1 eV, respectively. The valence band spectra of Alq$_3$/Nb:STO sample was measured *ex situ* by synchrotron-radiation photoemission system installed at BL2C at photon energy of 600 eV with an energy resolution of 0.25 eV. The film thicknesses were calibrated by *ex situ* grazing incidence X-ray reflectivity measurements.

Results and discussion

The valence band spectrum show systematic changes with increasing the Alq$_3$ film thickness, and finally become bulk Alq$_3$ spectra at 14-nm thickness. The several distinct peaks originated from Alq$_3$ molecular orbital (MO) were clearly observed and these energy positions

were in good agreement with the MO calculation [2]. In the 14-nm thick film, highest occupied molecular orbital (HOMO) onset was located at located at 2.2 eV below Fermi level. The difference of work function between Alq$_3$ and Nb:STO was estimated to be 0.6 eV from secondary electron emission spectra. Furthermore, corresponding peak shift was observed in core level spectra with increasing the Alq$_3$ thickness. From these experimental results, we determined the band diagram of the Alq3/Nb:STO interface as shown in Fig. 1, and found the formation of interface dipole with 0.6 eV.
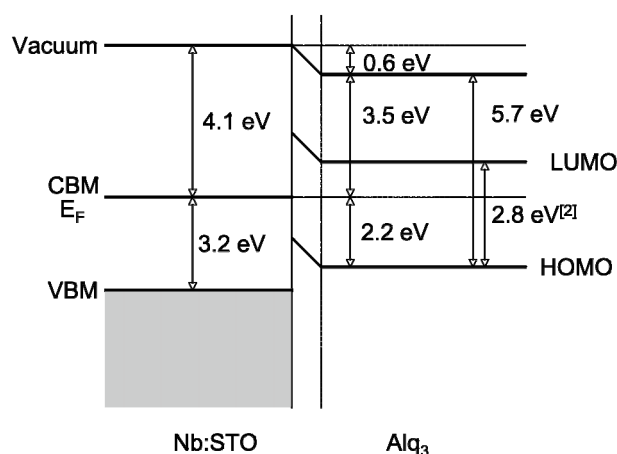

Fig. 1. Band diagram of an Alq$_3$/Nb:STO interface. The value of the band gap for Alq$_3$ were referred to that in Ref. 2.

References
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