Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Theoretical Investigation on the Electronic Structure of Alq3/Al Interface SUSUMU YANAGISAWA, Osaka University, YOSHITADA MORIKAWA, Osaka Univ., RICS-AIST — Alq_3 [tris-(8-hydroxyquinolinato) aluminum] is one of the most widely used electron transport and emissive material in organic light-emitting devices (OLEDs). From the experimental observation of an extra gap state at the Alq_3/Al interface, a strong chemical interaction between the Alq_3 molecule and the Al surface was suggested. Contrary to the experimental studies, previous DFT calculations concluded that the interaction was physisorptive. One possible reason for the discrepancy between the theoretical and the experimental results is the complexity of the experimentally used electrode surfaces. In the present study, we investigated the effect of the surface roughness on the electronic properties of the Alq_3/Al interface by examining various possible electrode structures. We examined three structures for the Al substrate, the flat Al(111) surface, the Al(332) stepped surface, and the Al adatom adsorbed Al(111) surface. Alq_3 molecules are bound to Al substrates through their O atoms and about 0.3-0.6 electrons are transferred from the Al substrates to Alq_3. Upward configurations, in which molecular permanent dipole moments are directed to the vacuum side, reduce the work function by 1.0-1.5 eV, in reasonable agreement with experimental results. The characteristic of the molecular orbitals of Alq_3 were kept upon adsorption, which seems inconsistent with the gap state derived from the interfacial chemical interaction observed in the UPS and MAES experiments. Further details will be presented.

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Date submitted: 01 Dec 2004 Electronic form version 1.4