

## Interfacial Electronic Structure of Bathocuproine and Al: Theoretical Study and Photoemission Spectroscopy

Jeihyun Lee, Hyein Kim, Dongguen Shin, Younjoo Lee, Soohyung Park, Jisu Yoo,  
Junkyeong Jeong, Gyeongho Hyun, Kwangho Jeong, Yeonjin Yi

Institute of Physics and Applied Physics, Yonsei University

Interfacial electronic structure of bathocuproine and Al was investigated using in-situ photoemission spectroscopy and density functional theory (DFT) calculations. Bathocuproine is used for exciton blocking and electron transport material in organic photovoltaics and Al is typical cathode material. When thin thickness of Al was thermally evaporated on BCP, gap states were observed by ultraviolet photoemission spectroscopy. The closest gap state yielded below 0.3 eV from Fermi level. By x-ray photoemission spectroscopy, interaction of Al with nitrogen of BCP was observed. To understand the origin of gap states, DFT calculation was carried out and gap states was verified with successive calculation of interaction of Al and nitrogen of BCP. Furthermore, emergency of another state above Fermi level was observed. Remarkable reduction of electron injection barrier between Al and BCP, therefore, is possible.

**Keywords:** BCP, photoemission spectroscopy, DFT, interfacial electronic structure