

Abstract Submitted
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Theoretical study on electronic structure of bathocuproine: Renormalization of the band gap in the crystalline state and the large exciton binding energy¹ SUSUMU YANAGISAWA, Department of Physics and Earth Sciences, Univ. of the Ryukyus, SHIN-NO-SUKE HATADA, YOSHITADA MORIKAWA, Department of Precision Science and Technology, Osaka Univ. — Bathocuproine (BCP) is a promising organic material of a hole blocking layer in organic light-emitting diodes or an electron buffer layer in organic photovoltaic cells. The nature of the unoccupied electronic states is a key characteristic of the material, which play vital roles in the electron transport. To elucidate the electronic properties of the molecular or crystalline BCP, we use the GW approximation for calculation of the fundamental gap, and the long-range corrected density functional theory for the molecular optical absorption. It is found that the band gap of the BCP single crystal is 4.39 eV, and it is in agreement with the recent low-energy inverse photoemission spectroscopy measurement. The polarization energy is estimated to be larger than 1 eV, demonstrating the large polarization effects induced by the electronic clouds surrounding the injected charge. The theoretical optical absorption energy is 3.68 eV, and the exciton binding energy is estimated to be 0.71 eV, implying the large binding in the electron-hole pair distributed around the small part of the molecular region.

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