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Aluminium as efficient hole-collecting electrode for active layers in inverted architecture photovoltaic devices

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Abstract

Inorganic-organic heterojunctions exhibit promising properties for various applications, including sensors, light-emitting diodes, and photovoltaic devices. Important factors of device performance and efficient charge transfer, strongly depend on alignment of energy levels between the metal electrode and the organic layer. Properly tuned energy barriers facilitate charge carrier transport across the interface, enhancing charge injection or extraction. Even a minimal number of interlayers, can significantly impact the energetic landscape at the contact. A deliberate selection of materials that enables the elimination of additional interfacial alignment layers can simplify the fabrication process while simultaneously improving device performance.

Current research in the photovoltaic field concentrates on inverse structure, which often exhibits better stability because the hole-collecting electrode (metal) is shielded from direct exposure to environmental factors. In the literature, the greatest interest of researchers is focused on aluminum, mostly, employing as a cathode due to its low work function (~4.1–4.3 eV).[1] Aluminum electronic properties can be modulated through surface modification, interfacial engineering, or controlled oxidation. These changes enable to match the energetic alignment of the HOMO level of donor-type active layers. Intsights into the interfacial energy level alignment and charge transport mechanism of aluminum/organic interfaces are therefore critical for optimizing junction performance as a hole-collecting contact in high-efficiency devices.

In this study, we investigate inorganic–organic complexes based on phthalocyanines deposited onto aluminum substrates via physical vapor deposition. To characterize the interfacial properties, surface-sensitive techniques such as X-ray Photoelectron Spectroscopy (XPS) and Ultraviolet Photoelectron Spectroscopy (UPS) were employed, providing insight into the core level positions, chemical composition, and valence band alignment.

To theoretically argue the selection of phthalocyanine compounds, calculations based on quantum chemistry were performed to determine the Density Of States (DOS) and initial electron properties. The simulations were carried out using Density Functional Theory as implemented in the Quantum ATK software, enabling accurate and computationally efficient analysis.

Based on the obtained data, a comprehensive band structure diagram of the full system was constructed.

References

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