Ex-Situ XANES/EXAFS for Chemical Structure Investigation of CIS/ZnCdS Photoanode in QDSSC Devices

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Abstract

The proper use of surface passivation layer in quantum dot (QD)-sensitized solar cells (QDSSCs) plays a crucial role in preventing surface charge recombination and, thus, improving the overall power conversion efficiency (PCE). In this work, we introduced a novel and facile ternary (CdZnS) passivation layer to enhance the photovoltaic performance of QDSSCs. Consequently, the device exhibits remarkably enhanced short-circuit current (JSC), open-circuit voltage (VOC), fill factor (FF), and power conversion efficiency (PCE). The QDSSCs with a CdZnS passivation layer confirmed strongly inhibited interfacial charge recombination and greatly enhanced light harvesting, resulting in a PCE of up to 8.83%, which is appreciably higher than 7.17% for the solar cells with a ZnS passivation layer and 3.99% for the solar cells without a passivation layer. In this regard, the phase determination, local inter-atomic distances, and distortion estimated by extended X-ray absorption fine structure (EXAFS) and X-ray absorption near-edge structural (XANES) spectroscopies. In fact, fine structures and the atomic arrangement regarding bond distance and coordination number were studied to identify metals neighbor and oxidation states along with the electrochemical nature and corrosion mechanisms before and after applying different passivation layers. Together with the PCE and electrochemical impedance spectroscopy (EIS) results, XAS studies revealed the underlying mechanism of the improvement of photovoltaic performance.

Keywords – XANES/EXAFS, QDSSCs, Ternary passivation layers, CdZnS.