Nanoscale chemical analysis of Sb_2Se_3 solar cell using tip-enhanced Raman spectroscopy

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class="Standard1">Among second-generation solar cells, Sb_2Se_3-based cells have gained great interest due to their lack of toxicity, higher abundance of Sb_2Se_3 compared to the conventional absorber materials, and highest reported power conversion efficiency (PCE) of 9.2%.[1] The Sb_2Se_3 solar cell is doped with copper and consists of a layered structure, which is shown in Figure 1a. The chemistry and structure of the interface between the layers plays a key role in determining efficiency. At the layer interfaces, chemical defects such as newly formed compounds or structural defects such as inhomogeneous layer separation can critically influence PCE.

Since the interfacial regions in these solar cells have nanoscopic dimensions, their analysis requires a nanoanalytical tool because when using conventional analytical techniques such as confocal Raman spectroscopy, the information from the individual layers averages out, precluding nanoscale analysis. In this study, we demonstrate that tip-enhanced Raman spectroscopy (TERS)[2] is a sensitive analytical tool for non-destructive nanoscale chemical characterization of interfacial regions in solar cells under ambient conditions.

By investigating a Sb_2Se_3 thin film solar cell, we show that TERS imaging can be used to probe this type of solar cell with a spatial resolution of up to 10 nm (Figure 1b). Interestingly, the two layers (Sb_2Se_3 and CdS) do not appear completely separated, as some areas in the Sb_2Se_3 layer show a strong CdS signal (blue pixels in Figure 1b). In addition, high-resolution TERS imaging revealed some regions with bands, which could not be assigned to either Sb_2Se_3 or CdS, indicating the presence of some unknown defects/impurities in these layers.

In summary, this study demonstrates the potential of hyperspectral TERS imaging to investigate defects/inhomogeneities in the interfacial regions of novel solar cells with nanoscale resolution.

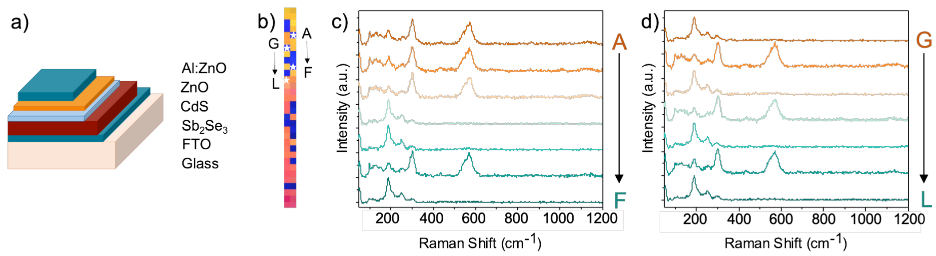

Figure 1 a) Scheme of the layer structure of a Sb_2Se_3 solar cell. b) Overlay of the Raman images generated by the intensity of the CdS Raman band (300 cm^{-1}, blue) and Sb_2Se_3 Raman band (190 cm^{-1}, red) and the oxidized Sb_2Se_3 Raman band (250 cm^{-1}, green). Size: 640 × 20 nm^2. c) Raman spectra were measured along the black arrow A-F marked in Panel b. d) Raman spectra were measured along the black arrow G-L marked in Panel a. All spectra were background subtracted and smoothened. Laser power: 263 µW. Acquisition time: 5 sec. Step size: 10 nm.

[1] Li et al., *Nat. Commun.*, **2019**, 10, 1-9.

[2] Cai Z., Kumar N., Zenobi R., *CCS Chem*, **2023**, 5, 55–71.