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Intrinsic defects and passivation mechanisms in Al_2O_3 ALD films

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The characterization of intrinsic defect mechanisms in Al_2O_3 thin films is essential for their effective use in surface passivation schemes for solar cells. Particularly, perovskite solar cells (PSC) have shown an enhanced long-term stability and an improved protection against ambient conditions when an ALD-Al_2O_3 layer is introduced into the PSC stack [1].

In this work, we discuss comparatively ALD-Al_2O_3 films prepared on different substrates (including MAPI: $CH_3NH_3PbI_3$) and by different process parameters (thermal-ALD, plasma-enhanced-ALD, substrate temperature). These films were analyzed by resonant photoelectron spectroscopy.

Intrinsic defect states within the electronic band gap were observed including excitonic, polaronic, and charge-transfer defect states, where their relative abundance depends on the choice of the used ALD parameters and substrate [2,3]. The most pronounced signature of excitonic states is found for the Al_2O_3 film prepared on MAPI at room temperature. It points to a strong distortion of the octahedral coordinated network with a high number of tetrahedral sites which have a high affinity for OH adsorption and, hence, are responsible for perovskite protection against humidity [2].

[1] M. Kot et al., ChemSusChem 9 (2016) 3401.

[2] K. Henkel, M. Kot, D. Schmeißer, J. Vac. Sci. Technol. A 35 (2017) 01B125.

[3] K. Henkel, M. Kot, M. Richter, M. Tallarida, D. Schmeißer, in K. Wandelt (Ed.): Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry, Elsevier, Oxford, 2018, vol. 3.1, pp 18-26.