PhD THESIS DEFENSE: Fluorescence quantum yield and the open circuit voltage in perovskite solar cells

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To mitigate the energy and climate crisis we are already facing and address the increasing energy consumption, it is essential to foster energy transition strategies. The energy transition success largely depends on being able to transform the global energy sector from fossil fuel-based to neutral or zero carbon dioxide emission sources. A decades-long study of photovoltaics has produced several generations of solar energy conversion technologies that do not emit greenhouse gases or air pollution when they operate. However, considering the sun is our planet's most abundant energy source, when compared to fossil fuels, the use of photovoltaics is still very limited. In such a transition from fossil fuels to photovoltaics, it is essential to enhance affordability combined with high efficiency. In recent years, perovskite solar cells have emerged as the most prominent thin-film PV technology to provide high

efficiency simultaneously at a low cost. In this thesis, we study perovskite-based solar cells and optical routes to maximise their power conversion efficiency. The theoretical limit for converting sunlight into electricity by the photovoltaic effect was first established by William Shockley and Hans-Joachim Queisser in 1961 based on the principle of detailed balance. According to their work, a solar cell can reach a limiting efficiency if all loss mechanisms are eliminated and the fluorescence quantum yield is equal to unity. The conversion efficiency for all PV technologies is still considerably lower than the Shockley - Queisser efficiency limit, but perovskite-based ones have demonstrated outstanding optoelectronic properties and high fluorescence quantum yields, which may help get their maximum PV efficiency closer to such limit. In this thesis, we provide several optical routes to optimise the photovoltaic parameters of perovskite solar cells, placing a special emphasis on the open circuit voltage by studying its relation to the absorption and emission of photons by the perovskite layer. This thesis is organised into five chapters. Chapter 1 serves as an introduction, which includes a discussion of the current world energy demand and available photovoltaic technologies, focusing more on the ones based on perovskite materials. The Shockley - Queisser efficiency limit and power loss mechanism are also described in this chapter. In Chapter 2, we analyse the relationship between open circuit voltage and fluorescence quantum yield in perovskite-based solar cells, both theoretically and experimentally, and discuss the observed deviation from the predicted behaviour. Chapter 3 describes the new fabrication method of high-quality perovskites with low band gaps and big grain size is described. The two-step compact PbI2-templated growth method facilitated the achievement of solar cells with high fluorescence quantum yield and open circuit voltage. In Chapter 4, we developed a model and optimisation algorithm to find the optimum photonic structures to optically enhance the photovoltaic parameters for different band gap perovskite solar cells. Theoretical results from this chapter suggest that a simple dielectric multilayer placed on top of the substrate of the solar cell can simultaneously improve the open circuit voltage and short circuit current, resulting in a relative gain of power conversion efficiency larger than 4%. Finally, in Chapter 5, the concept theoretically studied in the previous chapter is experimentally implemented. The dielectric multilayer is fabricated and placed on top of a perovskite solar cell, resulting in an enhanced open-circuit voltage and power conversion efficiency.

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