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Guiding safe and sustainable technological innovation under uncertainty: a case study of III-V/silicon photovoltaics

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Summary

This thesis aimed to address the main challenge in the environmental appraisal of emerging technologies to guide safe and sustainable innovation: the uncertainty about future developments which can influence the technology's environmental performance. While uncertainty may be regarded as an 'inconvenience' to conducting meaningful appraisals, this work offers an upside to the inconvenience in that it can be an important source of opportunities for safer and more sustainable designs. This work is motivated by the view that safety and sustainability assessments cannot fall behind to technological or economic drivers of innovations, which already rely on sophisticated methods to deal with uncertainties in these domains. Thus, the overarching aim of this work was to bring forward the practice of ex-ante/prospective life cycle assessment and risk assessment of emerging technologies by relying on novel adaptations of uncertainty analysis and global sensitivity analysis.

In Chapter 1 we introduced the pressing need and challenges in conducting environmental appraisals of technologies while they are still at early research and development stages. We showed how this is especially relevant for emerging photovoltaics (PV) which have seen accelerated growth in deployment and innovation in the past decades. We also introduced the case study of multijunction III-V/silicon tandem solar cells, a promising high-efficiency solar cell design for which no environmental assessments had been conducted prior to this work.

In Chapter 2 we surveyed the PV innovation landscape to investigate whether innovation in the sector as a whole was leading to reduced environmental impacts, as well as to identify environmental hotspots across the proposed technologies. For this we conducted a systematic review and meta-analysis of life cycle assessment (LCA) studies of emerging PV technologies in the period 2010-2020. In most cases, the impacts of emerging PV were lower on average than those of the incumbent technology in 2010, Al-BSF c-Si cells. However, due to large variabilities and heterogeneity we found no discernible trend in time or statistically significant effect of innovation on climate change impact scores. Of the technologies surveyed, most hotspots were found in perovskites vs. other technologies. These hotspots could be mostly attributed to the fluorine-doped tin oxide (FTO) glass component. Life cycle impacts of perovskite cells were magnified because of the perovskite cells' short lifetimes.

In Chapter 3 we conducted a comprehensive LCA of a lab/pilot scale version of the III-V/Si tandem solar cell technology. At this scale, III-V/Si was found to perform better than the Al-BSF c-Si cells which dominated the market until 2015, but slightly worse than PERC c-Si cells which have dominated since. However, our break-even analysis concluded that foreseeable optimizations in energy reduction and/or increased throughput in the MOVPE process could lead to an advantage in environmental performance of III-V/Si over state-of-the-art PERC c-Si cells.

In Chapter 4 we proposed and successfully demonstrated two important modelling enhancements needed to assess technologies beyond lab/pilot scale in an *ex-ante* LCA framework. First, unresolved choices of materials or processing methods (referred to as *technological pathways*) were modelled using binomial distributions which trigger the pathways

stochastically depending on their chances of success. Second, a novel screening algorithm was developed to allow a global sensitivity analysis (GSA) to be conducted on full-scale LCA models with an unprecedented number of uncertain model inputs, including unresolved technological pathways. The joint application of both enhancements to emerging front metal designs for PV cells allowed us to discern which unresolved technological pathways would be the most influential on the cells' future environmental performance. In this case, the choice between laser and chemical sintering methods for the copper ink, and the choice between silver and copper ink were considerably more influential than all other choices.

In Chapter 5 we conducted a prospective ecological risk assessment of the III-V/Si PV technology for high-electrification/high PV demand scenarios in three geographical scales: Europe, Amsterdam region, and a local utility-scale plant. The emissions and risks from III-V/Si PV cells were found to be low in worst-case situations, and negligible in other cases. A GSA identified operational parameters in the landfill end-of-life route as the most influential factors (waste/leachate partitioning and landfill cell depth). These factors were taken as a basis to produce recommendations for safe-by-design of III-V/Si PV panels and ancillary systems, such as increased separation for reuse of the III-V layers, substitution of the ethyl vinyl acetate (EVA) encapsulation for less acid-generating materials, and more vertical landfill cell designs.

Chapter 6 built on the experiences and insights from the previous chapters to propose a generalized framework for *ex-ante*/prospective assessments to guide safe and sustainable innovation. We showed that GSA can be used as a screening tool to identify the most influential factors across different domains (e.g., economic, social, technological, environmental). A hierarchy of risk mitigation strategies was proposed to target these influential factors at the design stage. For the III-V/Si cells we found that, once all foreseeable improvements in cell design and manufacturing are applied, extending the useful life of the panels and/or avoiding early obsolescence can offer the most effective impact reduction strategy. In this chapter we also demonstrated for the first time how the Bayesian approach to probability can be applied and may be better suited than the frequentist approach to deal with uncertainties in *ex-ante*/prospective assessments. We also showed how simple analytical solutions can be used to perform Bayesian inference and further reduce uncertainty on the influential factors identified.

In Chapter 7 we finalized by discussing the strengths of the ex-ante/prospective approach developed in this work, in that it can focus resources much more effectively than approaches relying solely on potentially biased scenario analysis. We also highlight how this approach provides a more transparent way to make design choices in light of numerous underlying assumptions and residual uncertainties.