

# Materials and Device modelling in Emerging Inorganic Chalcogenides for Photovoltaics

## Summary

*Defects have a strong impact on the performance of thin film absorber materials and solar cells. We are looking for a candidate to work on the theoretical modeling of materials ( $\text{Sb}_2\text{Se}_3$ ,  $\text{Sb}_2\text{S}_3$ ,  $\text{Bi}_2\text{S}_3$ , and their related alloys) and solar cell devices, with the goal of supporting, guiding, and accelerating experimental development. This work will require the use of ab initio density functional theory (DFT) techniques, as well as drift-diffusion models for simulating charge transport in thin-film solar cell structures, along with other relevant modeling approaches. As the research group currently lacks dedicated expertise in theoretical modeling, the successful candidate will become the in-house expert in this area, offering a unique opportunity to establish an independent research platform while working closely with the experimental team and gaining hands-on experience with a range of physical and chemical thin-film deposition techniques. The candidate will join a diverse and collaborative research environment, with the opportunity to be actively involved in the COST Action CA21148 – ReNewPV. Through this network—and specifically via the dedicated Materials and Device Modeling Working Group in ReNewPV—we will ensure strong collaborative ties (including potential joint supervision) between the Laboratory for Thin Film Energy Materials at TalTech (Tallinn, Estonia), the Photovoltaic Group (Prof. Dr. Zacharie Jehl Li-Kao) at the Department of Electronic Engineering, Polytechnic University of Catalonia (UPC – BarcelonaTech), and the group of Prof. Keith McKenna at the University of York, UK, who also leads Working Group 2 in ReNewPV. The successful applicant will have a unique opportunity to conduct research visits (Short-Term Scientific Missions) at UPC, the University of York, and other collaborating institutions.*

Research field:	Chemical, materials and energy technology
Supervisor:	Dr. Nicolae Spalatu
Availability:	This position is available.
Offered by:	School of Engineering Department of Materials and Environmental Technology
Application deadline:	Applications are accepted between June 01, 2025 00:00 and June 30, 2025 23:59 (Europe/Zurich)

## Description

**Eligibility / Qualifications-** The research group *Laboratory for Thin Film Energy Materials* at TalTech is seeking excellent and highly motivated candidates who hold, or are about to complete, a Master's degree in Physics, with a strong background in Materials Science, Solid-State Physics, and Computational Physics. Previous experience in thin-film and solar cell characterization, as well as materials and device modeling, will be considered a big advantage. An excellent team-working attitude and strong communication skills in English (both written and oral) are essential requirements. Competence in data analysis and graphing software—such as Microsoft Office (Word, Excel, and PowerPoint) and Origin—is also expected.

**Research Profile of the Group** - The R&D portfolio of the research group focuses on the development of emerging inorganic chalcogenide thin-film photovoltaic (PV) technologies for specialty PV markets, including building-integrated photovoltaics (BIPV), product-integrated photovoltaics (PIPV), PV-powered IoT applications, and future green responsible optoelectronics. During the last years, the group's primary research has centered on the development of novel thin-film PV materials and solar cells based on,  $\text{Sb}_2\text{S}_3$ ,  $\text{Sb}_2\text{Se}_3$ ,  $\text{Sb}_2(\text{S,Se})_3$ ,  $\text{Bi}_2\text{S}_3$  and their related solid solutions/alloys, using both physical vapor deposition (PVD) and chemical methods. These include close-spaced sublimation, vapor transport deposition, spray pyrolysis, chemical bath deposition, and sol-gel processing. The technologies developed in the laboratory are designed to be simple, cost-effective, and readily scalable for industrial implementation.

The laboratory team actively coordinates and participates in several international and national research projects. They are also the Grant Holder institution for the COST Action *RENEW-PV*—a global network of over 400 researchers and industrial partners from more than 50 countries, dedicated to the advancement of emerging inorganic PV materials and devices, <https://renewpv.eu/>.

## Responsibilities and (foreseen) tasks

- Identify problematic intrinsic and extrinsic defects in device layers, giving relevant information for the design of defect passivation strategies for device performance optimization.
- Provide analysis of performance limiting effects at interfaces including mitigation strategies.
- Perform device level simulations based on simulated and experimentally determined materials properties to predict device performance optimisation routes and identify bottlenecks.
- Analysis of the research data, preparing reports, oral and/or poster presentations at conferences, publishing research articles.

**How to Apply-** Applications should include a motivation letter, the contact details of two references, a full curriculum vitae (CV), and copies of relevant diplomas with transcripts of grades. Applicants should also submit a brief research plan related to the topic, demonstrating their understanding of the current state of the art in the proposed field and outlining a proposed plan of research activities.

Main supervisor: Prof. Nicolae Spalatu

Co-supervisor: Prof. Zacharie Victor Samuel Nathanaël Jehl

**We offer:**

- 4-year PhD position in one of the most internationalized and leading PV research groups in Estonia
- The chance to do high-level research in one of the most booming emerging photovoltaic field.
- Opportunities for conference visits, research stays and networking with globally leading universities and research centres in the fields of material science.
- Opportunity to be part of the COST action CA21148 - Research and International Networking on Emerging Inorganic Chalcogenides for Photovoltaics, RENEW-PV, <https://renewpv.eu/>

**Contact** – For further information, please contact Prof. Nicolae Spalatu [nicolae.spalatu@taltech.ee](mailto:nicolae.spalatu@taltech.ee) and Prof. Ilona Oja Acik [Ilona.oja@taltech.ee](mailto:Ilona.oja@taltech.ee), or visit <https://taltech.ee/en/laboratory-thin-film-energy-materials>



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