

Accelerated experiments on 25,000 solar-relevant semiconductors with chalcogenide and pnictide anions

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We have been studying exotic semiconductor systems with a focus on mixed-anion compounds with experimentally challenging anions, such as phosphosulfides, phosphotellurides, and sulfonitrides¹. Previous reports of thin-film synthesis in these exotic systems are essentially non-existent. This lack of experimental studies is unfortunate, because these material families have a remarkable degree of chemical diversity that could enable exciting applications in photovoltaics, photoelectrochemistry, and beyond².

Aided by a combinatorial, multi-technique thin-film deposition setup, we have now synthesized 25,000 unique samples from these exotic systems³, including several single-phase semiconductors not reported before as thin films, with clear potential for PV, PEC, or as transparent conductors. Detailed growth and characterization data from many of these samples is already publicly available at <https://nomad.nanolab.dtu.dk/nomad-oasis/gui/search/combinatorial-samples>.

In this seminar, I will reflect on the properties of the synthesized materials, the lessons learned from these accelerated materials discovery campaigns, and broad cross-chemistry trends in synthesizability and properties enabled by the large volumes of collected data. The synthesized materials include: the Cu₃PS₄ thiophosphate with many similarities to CIGS but lower growth temperature⁴; the BaP₄Te₂ phosphotelluride with ideal properties as a top absorber for tandem PV; the Zr₂N₂S sulfonitride showing promise both as a p-type transparent conductor and as a light-trapping layer in solar cells⁵; the BaZrS₃ perovskite featuring photoluminescence and photoconductivity at low growth temperatures⁶; and the defect-tolerant BaCd₂P₂ Zintl phase recently discovered by computational methods but that had so far eluded thin-film synthesis.

1. Sanz Rodrigo, J. *et al.* Machine-Learning-Assisted Discovery and Accelerated Synthesis of Metal Phosphosulfides. *Small* **22**, e74742 (2026).
2. Mittmann, L. A. & Crovetto, A. Phosphosulfide semiconductors for optoelectronics and solar energy conversion. *J. Phys. Mater.* **7**, 021002 (2024).
3. Mittmann, L. A. *et al.* Digital infrastructure to support and share daily high-throughput experimental materials research. *Faraday Discuss.* <https://doi.org/10.1039/d6fd00019c> (2026)
4. Mittmann, L. A. *et al.* Large-area thin-film synthesis of photoactive Cu₃PS₄ thiophosphate semiconductor with 0–14 pH stability range. *Chem. Sci.* **16**, 21862–21873 (2025).
5. Bertin, E. *et al.* A sulfonitride transparent conductive thin film with ultra-high refractive index. <https://doi.org/10.48550/arXiv.2605.22483> (2026).
6. Itzhak, A. *et al.* Photoluminescent and photoconductive BaZrS₃ films grown at device-compatible temperatures from stable sulfide precursors. <https://doi.org/10.26434/chemrxiv.15006097/v1> (2026).

Bio

Andrea Crovetto leads the Thin Film Materials Discovery group at DTU Nanolab, Technical University of Denmark. He was previously a Marie Skłodowska-Curie fellow at the National Renewable Energy Laboratory (USA) with Andriy Zakutayev, and at Helmholtz Zentrum Berlin (Germany) with Thomas Unold. The focus of Andrea's research is the discovery and understanding of thin-film materials from unusual nooks of the periodic table. His key application area is optoelectronics, including solar cells, electrochemical cells, and transparent conductors.