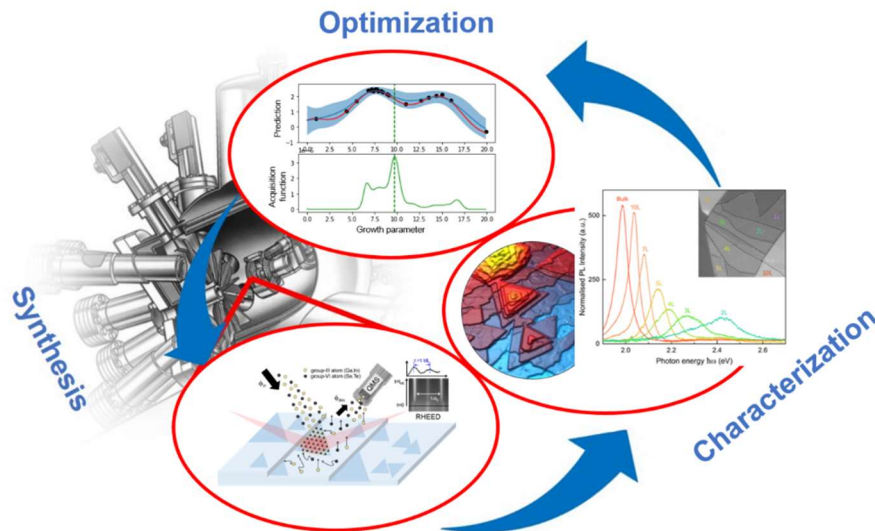


## MSc topic on "Machine-learning aided optimization of MBE grown ultrathin 2D Gallium Selenide (GaSe)"



Novel 2D materials “beyond graphene” have sparked immense interest in recent years, due to their excellent tunability, efficient light-matter coupling, and miniaturization capabilities. In our group, we study the epitaxial growth of 2D-material nanostructures by molecular beam epitaxy (MBE), a technique known for the scalability and superior controls of all three thickness, interface and defect, which are fundamental conditions for standard device fabrication, with a special focus on the group-III-monochalcogenides(III-MCs)/nitrides. In particular, this project aims at investigating the synthesis of 2D-GaSe, a III-MC material having unique optoelectronic properties [1], in a cutting edge 2D-MBE-Analytic cluster.

You will explore nucleation kinetics to identify phases, domain size and orientation in dependence of substrate preparation and growth parameters. The optimization step will employ a structured “design of experiments” (DOE) approach and will explore the implementation of Bayesian-Optimization-based machine learning algorithms [2], in order to speed-up the process. You will map prevalent growth modes and morphologies and tune the (opto)electronic properties in the few-layer regime of GaSe. The thesis will include working with many state-of-the-art surface science-based characterization techniques (RHEED, line of sight QMS, XRD, AFM, XPS, PFM) and spectroscopic techniques (PL, Raman, differential reflectivity).

While working on the project, you will learn about how to create and investigate a new material, explore the intriguing field of MBE and earn a deep understanding of process optimization, as well as UHV-technology.

We are seeking highly motivated, hardworking students with an inclination for technical and fabrication lab work. Some experience with epitaxial growth, optical spectroscopy, 2D materials, scripting (Python) will be beneficial but not essential.

If you are interested to become part of our research team, please send your CV, transcript of your records and Bachelor thesis to Dr. Eugenio Zallo ([eugenio.zallo@wsi.tum.de](mailto:eugenio.zallo@wsi.tum.de)), Michele Bissolo ([Michele.Bissolo@wsi.tum.de](mailto:Michele.Bissolo@wsi.tum.de)) and Prof. Jonathan J. Finley ([finley@wsi.tum.de](mailto:finley@wsi.tum.de)).

[1] H. Cai, et al., “Synthesis and emerging properties of 2D layered III-VI metal chalcogenides”, Appl. Phys. Rev. 6, 041312 (2019).

[2] Wakabayashi, Y. et al. "Machine-learning-assisted thin-film growth: Bayesian optimization in molecular beam epitaxy of SrRuO<sub>3</sub> thin films", APL Materials 7, 101114 (2019).