Physik der Molekularen und Biologischen Materie

Arbeitsgruppe Prof. Dr. Frank Schreiber

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Master and Bachelor Project:
Machine Learning for Fast Analysis of Scattering Data

Project description:

Using today's computing power and software packages it has become possible to analyze large and multi-dimensional experimental scattering data. The process of converting these data into useful scientific information, however, can be challenging. Popular machine learning models, such as artificial neural networks, have recently shown significant advantages in terms of speed over other computational methods that are usually employed to extract the essential parameters of the investigated systems.

Within the field of soft matter physics, our group studies the fundamental structural properties, particularly the growth process, of molecular thin films or perovskite solar cells [1,2]. In this context, we collect X-ray scattering data using highly specialized synchrotron beamlines, e.g. at the ESRF in Grenoble or at DESY in Hamburg. Modern area detector technology allows us to record enormous amounts of complex data, however, usually data analysis remains the bottleneck for the scientific output.

Therefore it is necessary to develop new and advanced tools for fast data analysis. In this specific project, you will

- develop new and improve existing machine learning models [3,4] in Python using common frameworks such as TensorFlow or PyTorch.
- perform computer-based modelling of scattering data, for instance X-ray reflectivity data or 2D scattering images, in order to generate high-quality training data for machine learning models,
- and compare the performance and prediction accuracy of these models to standard approaches such as least mean square fitting.

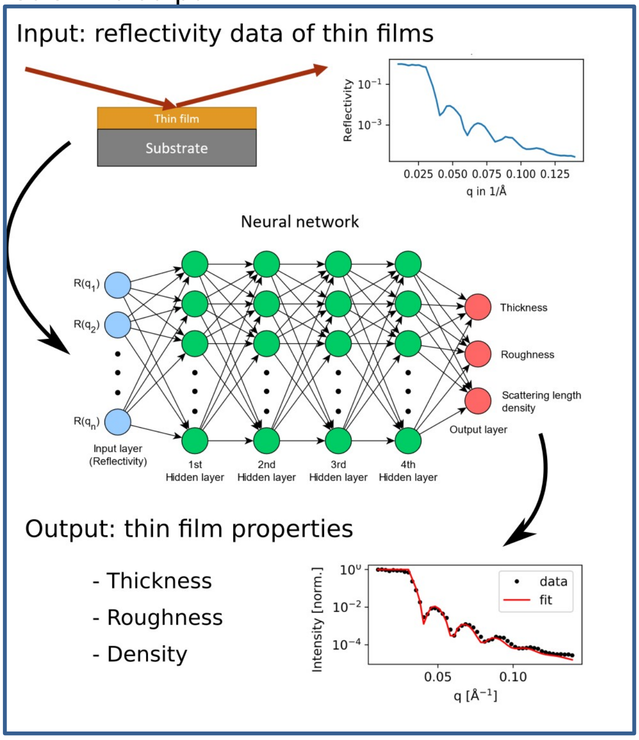

Figure: Using artifical neural networks to extract thin film properties from X-ray reflectivity data.

Starting time: ***immediately***

Candidates with a background in computational methods and programming with an interest in soft-matter physics are encouraged to apply for this project.

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References and further information:

www.soft-matter.uni-tuebingen.de (see under publications and open positions)

1. C. Frank et al., Phys. Rev. B **90** (2014) 205401
2. Y. Liu et al., Angew. Chem. Int. Ed. **59** (2020) 15688
3. V. Starostin et al., npj Comput Mater **8** (2022) 101
4. A. Greco et al., J. Appl. Cryst. **55** (2022) 362