A picture worth a thousand atoms: 2D image to 3D nanostructure mapping by merging simulated and measured data

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You probably know the saying a picture is worth more than a thousand words, but is that really always the case? What if the picture is blurry? What if what you're trying to capture is a complex three-dimensional structure, yet the picture only provides a two-dimensional snapshot from one angle? My name is Reinhard Maurer and I'm supervising a PhD project as part of the HetSys CDT that aims to tackle this issue in the context of imaging and characterization of nanostructures in two-dimensional materials. Materials characterization is being revolutionized by new spectroscopy and atomistically resolved imaging techniques, such as transmission electron microscopy. With resolution ever improving, we can better compare to atomistic simulation results and the challenge really becomes how to combine information from experiment and simulation.

For example, transmission electron microscopy, as shown here, gives us an integrated 2D image of a metal nanoparticle, but what is the real three-dimensional structure of the particle that defines this, its stability, properties, and reactivity, for example in catalysis? As part of this project, we will use electronic structure theory, such as density functional theory, and simulations to complement incomplete experimental data. With the help of machine learning models, we will aim to develop a mapping of 2D images to the most likely 3D nanostructures that could potentially give rise to that image. Our goal is to develop a structure prediction tool that is applicable to real experimental imaging data of nanomaterials, such as catalysts deposited on nanostructured graphene.

This project is co-funded by the Ada Lovelace PhD program of STFC and provides extensive training in scientific machine learning and electronic structure theory. You'll be supervised by a dream team of experts in theory, computation, and experiment, and you'll be able to go on secondments to STFC and Diamond Light Source, which is the national synchrotron facility. If this sparks your interest, please do get in touch.

Thank you.