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Machine-Learning Assisted Exit-wave Reconstruction for Quantitative Feature Extraction

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Reconstruction of the exit wave is a powerful tool to extract the maximal amount of information from High-resolution Transmission Electron Microscopy (HRTEM) [1,2]. In a recent publication, Chen et al. [3] used exit wave reconstruction to visualize the three-dimensional structure of cobalt doped Molybdenum Disulphide nanoparticles in a model catalyst. In addition to the three-dimensional structure of the nanoparticle, the reconstructed exit waves also contained information about the beam-stimulated vibrations of the atoms near the edge of the nanoparticle.

We have recently demonstrated that convolutional neural networks are able to reconstruct the exit wave from a focal series with a low number of images [4]. We train the neural networks on simulated images. The simulated images are produced with the multislice algorithm using the abTEM software [5], both the exit wave function and images produced with three different values of the defocus are saved. The neural network is then trained to reconstruct the exit wave from the images. The network is validated on a different set of simulated images, and if applicable applied to experimentally obtained data.

We demonstrated that it is possible to train neural networks to reconstruct the exit wave for a varied set of samples consisting of all structures in the Computational 2D Materials Database (C2DB) [6], see Figure 1. For a specialized dataset such as Molybdenum Disulphide (MoS_2) supported on graphene, a slightly lower error rate can be obtained (Figure 2), and realistic results can be obtained when the network is applied to experimental data [4].

In this work, we investigate how far the convolutional neural networks can be optimized towards obtaining quantitative information from experimental data, with a particular focus on the kind of data obtained by Chen et al. [3], i.e., reconstructing exit waves with sufficient accuracy to extract the three-dimensional structure and the amplitudes of the atomic vibrations. This can be realized with more flexible training sets than in our previous publication and by training the network to ignore the support when reconstructing the exit wave.

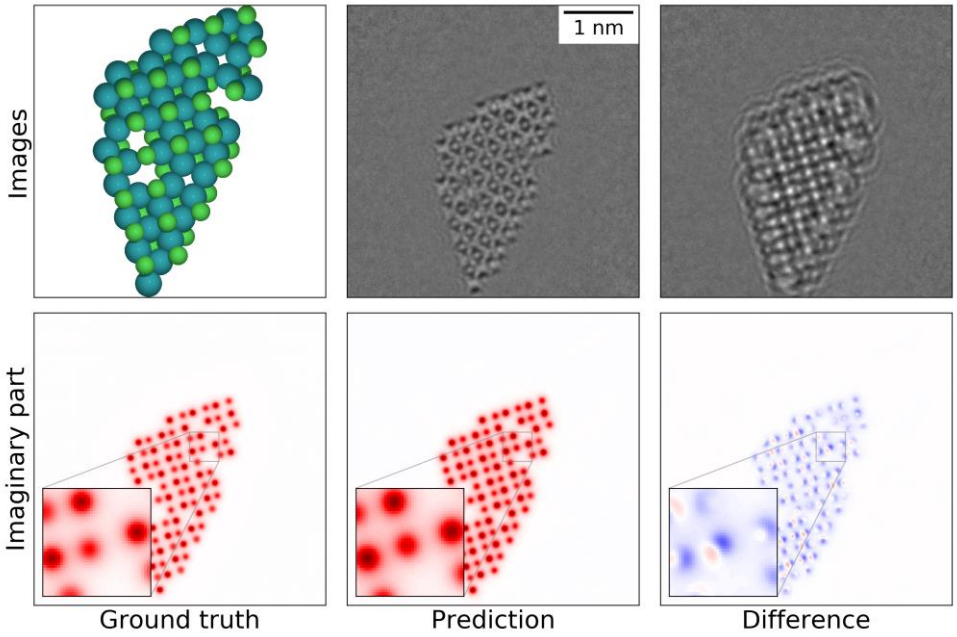

Figure 1. Rhodium Chloride, a sample structure from the C2DB database. The top row shows the structure and two of the three images used by the neural network. The second row shows the correct exit wave (the ground truth), the one predicted by the neural network, and the difference. Only the imaginary part is shown, as there is less signal in the real part. The network correctly locates all atoms, but it gets some of the positions slightly wrong, possibly due to the images being out of focus. Reproduced from reference 4, supplementary material.

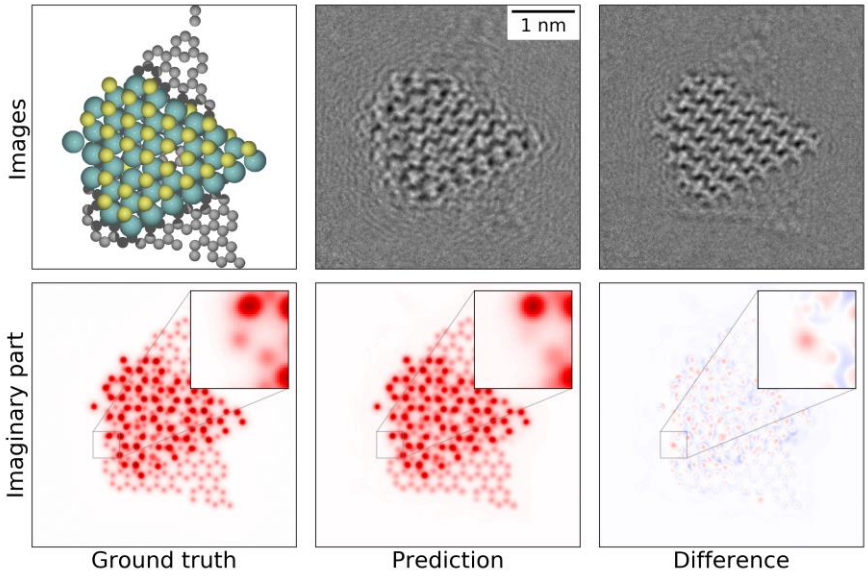

Figure 2. Molybdenum Sulphide on graphene. The network is partially missing a support atom which is simultaneously at the edge of the support and close to a molybdenum atom in the MoS_2 nanoparticle. Reproduced from reference 4, supplementary material.

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