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Chiral Structure Classification by a Convolutional Neural Network

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Scanning tunneling microscopy (STM) is an important tool to image surfaces at atomic scale, that allows to acquire significant amounts of data in comparably short time. Therefore, for example to examine large ensembles of molecules in STM images can be a difficult and time-consuming task. We present a method to recognize chirality within experimentally observed self-assembled molecular structures using the convolutional neural network (CNN) based object detection architecture YOLOv5. Thereby we classify unit cells in the image towards one of the two chiral orientations present on the surface.

To train the neural network, a sufficient amount of correctly labeled images is necessary. To obtain such data and labels, we utilize a method to create realistic-looking, synthetic STM images in varying zoom-sizes containing lifelike properties such as noise and defects along with corresponding labels.

Using this synthetic data, we trained a model capable of classifying synthetic images at sizes ranging from 8nm to 200nm with high performance. Evaluations of the CNN's predictions for real images show that this network trained on synthetic data can categorize chirality in real images.

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