

## Simulation of STM Surface Images from 3D Atomic Structures. A Unet-based Convolutional Networks Tool.

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While several programs exist for constructing TEM and STEM images from 3D atomic structures [1], simulating STM images is much more complex. It requires high level calculations for solving wave functions for both tip and sample, determining tunneling probabilities influenced by tip-sample interactions and bias voltage. STM is highly sensitive to many-body effects such as electron-electron correlations, local density of states variations, and phonon interactions, all of which are essential for high-fidelity simulations. Despite these challenges, STM is still widely used to characterize surfaces inaccessible to other methods such as 2D materials on a bulk substrate.

Post-processed DFT computed electronic wave function allow simulating STM images [2] which can be compared to experimental images to determine the surface morphology. However, solving the Schrödinger equation for large systems requires important computational resources, forcing a tradeoff between model size and accuracy. STM simulations are typically applied to 10-15 Å models, which are much smaller than experimental images. For example, STM imaging is used to identify borophene allotropes, but DFT comparisons rely on small models. [3-5] This approach confirms local atomic arrangements, but cannot capture large-scale organization, moiré patterns, or phase mixing within borophene deposits. [3-5]

We will present here a new tool based on the Unet convolutional network architecture [6] allowing to generate STM images of a material's surface from its 3D atomic structure. This tool takes as input an image and generate a new modified image. The input image is generated from a projection of atom's centered gaussian functions above the surface. The output image is the STM image obtained from a high level DFT calculations.

The tool has been developed and trained from hundreds of structures of various allotropes of borophene (extended layers and clusters) on a silver substrate surfaces. The structures have been generated from a previously developed Machine Learned Interaction potential (MLIP) [6-7] allowing a rather large variety of structural arrangements and thus STM images contrasts. Obtained images are in a very good agreement with DFT simulated ones which suggests potential use for other types of surfaces through future minor developments.

## References

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## Figures



**Figure 1.** STM imaging of  $\beta 8$  borophene allotrope on an Ag substrate. 3D structure (left) with B and Ag atoms in pink and grey, respectively. STM image simulation from DFT calculations (center) and the Unet-Tool (right).