Crossing the Simulation-Experiment Gap: Style Translation for Enhanced Atomic Structure Discovery from AFM Images

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Atomic force microscopy (AFM) is critical for characterizing atomic-scale structures. AFM simulations using particle probe model [1] provide a cost-effective approach for rapid AFM image generation. Using state-of-the-art machine learning models and substantial simulated datasets, properties such as molecular structure, electrostatic force potential, and molecular graph can be predicted [2, 3, 4] from AFM images. However, transferring model performance from simulated AFM to experimental AFM images poses challenges due to the subtle variations in real experimental data compared to the seemingly flawless simulations. In this study, we explore CycleGAN [5] for style translation to augment simulated images and improve the predictive performance of machine learning models in surface property analysis. We reduce the style gap between simulated and experimental AFM images and demonstrate the method's effectiveness in enhancing structure discovery models through local structural property distribution comparisons. This research presents a novel approach to improving the efficiency of machine learning models in the absence of labeled experimental data.

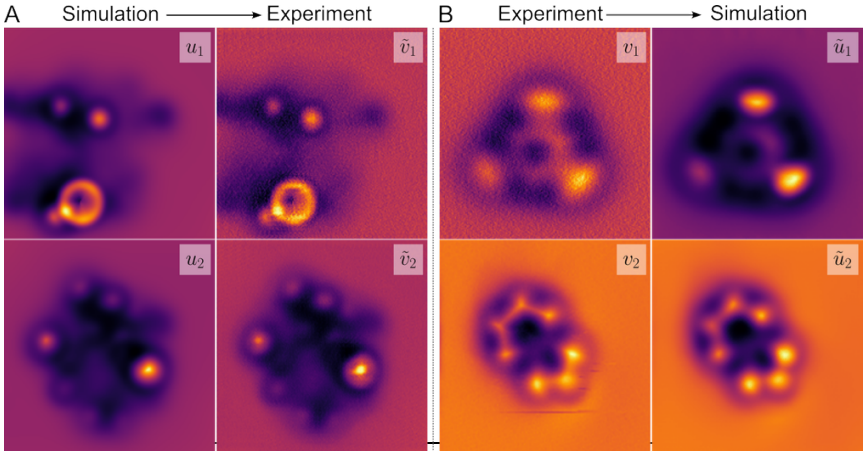

Figure 1. Style translations between simulated and experimental AFM images. Translated images in experimental style in improve model training over using simulated AFM images.

Reference

[1] N. Oinonen, et al., Comput. Phys. Commun. **305**, 109341 (2024).

[2] B. Alldritt, et al., Sci. Adv. **6**, eaay6913 (2020).

[3] N. Oinonen, et al., ACS Nano, **16(1)**, 89 (2022).

[4] F. Priante, et al., ACS Nano, **18(1)**, 1234 (2024).

[5] J.-Y. Zhu, et al., arXiv:1703.10593, (2020).