# Image Super Resolution for Scanning Tunneling Microscopy and Atomic Force Microscopy

Rockwell T. Li
Math and Science Academy
Ocean Lakes High School
Virginia Beach, VA, USA
rockwell.t.li@gmail.com

Marjorie Cenese
Department of Electrical Engineering
Old Dominion University
Norfolk, VA, USA
mcene001@odu.edu

Yuan Zhang
Department of Physics
Old Dominion University
Norfolk, VA, USA
y7zhang@odu.edu

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***Abstract*— Scanning Tunneling Microscope (STM) and qPlus Atomic Force Microscopy (Q+AFM) image nano-material surfaces at atomic level, which have led to many major scientific breakthroughs. However, their resolutions are often limited by realistic experimental conditions.**

**In this paper, we investigate image super resolution methods empowered by deep learning to go beyond STM and Q+AFM experimental limits. STM-SR and AFM-SR, adopting the Super-Resolution Generative Adversarial Networks (SRGAN) architecture, are developed and trained on high-resolution STM and Q+AFM datasets to convert low-resolution images into high resolution ones, respectively. Our results show that STM-SR and AFM-SR lead to significant resolution improvement compared to bicubic interpolation. This breaks the experimental barrier and reaches the resolution level near ideal conditions. This method can be applied to the study of large, complex molecules, which requires stringent experimental conditions.**

***Keywords—Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM), Single Image Super Resolution, Super-Resolution Generative Adversarial Networks (SRGAN)***

## I. Introduction

Scanning Probe Microscopy (SPM) [1] generates images by scanning the sample surface using a physical probe, which have over 1,000 times higher resolution in comparison with classical optical microscope. Scanning Tunneling Microscopy (STM) [2] and qPlus Atomic Force Microscopy (Q+AFM) [3] are well-established SPMs to image atomic-level surfaces and to probe material properties. These images reveal the geometry and electronic structures of the surfaces with atomic resolution. Since being invented, STMs and Q+AFMs have been responsible for many breakthroughs in nanophysics, material science, semiconductor science, and biochemistry [4].

The resolution of STMs and Q+AFMs is the most critical factor. High resolution STM or Q+AFM images can lead to precise measurement of physical properties, such as surface topography, electronic properties, strength of chemical bonds, dielectric and magnetic properties, and contact charges. Moreover, high resolution STM and Q+AFM scans enable the study of subtle effects in physics phenomena, including conformation changes, friction, lubrication, vibration, and molecular manipulation. STMs and Q+AFMs have a lateral resolution up to 0.1nm and a vertical resolution of 0.01nm [5, 6]. At this resolution, individual atoms within target samples can be routinely imaged. However, high-resolution atomic-level images are only achievable under ideal experimental circumstances, at cryogenic temperature, clean and stable surfaces, and sharp conducting tips. Oftentimes, due to limitations imposed by the target samples, experimental conditions cannot achieve high resolution. In particular, it is difficult to get atomic resolution when scanning large molecules at elevated temperatures, primarily because the high thermal energy causes significant mobility and movement of the molecules. Recently, experimental methods to enhance STM and Q+AFM resolution have been developed by functionalizing the scanning tip [7, 8] with an atom or a molecule (CO [9, 10], $H_2$ [11], $D_2$ [12], $CH_4$ [13], Xe [14], CuO [15], etc.) that significantly contributes to the tip-sample interaction, which can reveal the internal structure molecules adsorbed on surfaces. These experimental resolution enhancement methods have become successful in certain classes of molecules, and many astoundingly high-quality STM or qPlus AFM images have been generated. However, these experimental resolution enhancement methods based on functionalizing tips increased experimental complexity and are not universally applicable to any molecules of interest. The computational-based resolution methods, on the other hand, has great potential to complement the experimental methods.

The purpose of this paper is to demonstrate that the latest deep learning technology can computationally enhance the resolution of STM and Q+AFM images and overcome the physical limitations of STM and Q+AFM experiments. In this study, we model the STM and Q+AFM image super-resolution problem as a Single Image Super Resolution problem. We attempt to train deep learning models with many high-resolution images on a variety of molecules obtained from high-resolution STM or Q+AFM experiments to enhance the low-resolution images where the high-resolution versions cannot be obtained from experiments. Using a large set of high-resolution STM images across many molecule systems available as the training set, the STM-SR program adopts a Super-Resolution Generative Adversarial Networks (SRGAN) [16] architecture to transform low-resolution STM images into high-resolution STM versions. Similar mechanism is used to train AFM-SR on a collection of high-resolution Q+AFM images. Our STM-SR and AFM-SR results show that deep learning image super-resolution technologies can achieve a clearer view of the atomic world.

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## II. Background

### A. Scanning Tunneling Microscope (STM) and qPlus Atomic Force Microscope (Q+AFM)

STM works by scanning an extremely sharp metal wire tip over a surface of material samples with precise, angstrom-level control, taking advantage of the piezoelectric effect. When the tip is sufficiently close to the surface within sub-nanometer distance, the voltage bias between the tip and scanned surface enables electrons to tunnel through the vacuum in between to form tunneling current, due to quantum tunneling effect. As the tip encounters sample features of different heights, tunneling current changes correspondingly. Monitoring the tunneling current and coordinating the current with the positioning of the tip, the sample surface is imaged at the atom scale, resolving the conformations of individual atoms.

Q+AFM uses a tip mounted on a tuning folk that is driven to vibrate under its natural frequency to detect tip-sample interaction. The strength of such interaction is measured as a frequency shift from tip natural frequency. The measured frequency shift as a function of probe and surface distance can be calculated to form force image of the sample surface.

### B. Experimental Methods for STM and AFM Image Super-Resolution

Experimental methods by functionalizing the scanning tip has been developed to enhance STM and Q+AFM image resolution. The fundamental idea is that the resolution of STM or Q+AFM images crucially depends on the chemical nature of the sharp tip apex. Hence, functionalizing the scanning tips with a molecule or an atom can trigger the interaction between the tip and the specific structure of the target sample. Intentionally picking up the functionalizing molecule or atom amplifies the detected signal, which is the key to dramatically enhancing the resolution of STMs and qPlus AFMs. For example, functionalizing the STM tip with a single CO molecule improves the resolution of molecular orbital STM images [9, 10, 17]. Another example is the scanning tunneling hydrogen microscopy (STHM) with STM tip functionalization with H2, D2, and a variety of other atomic and molecular particles [11-15], which allows the STM to resolve the atomic structures of large organic adsorbates in a direct imaging experiment. AFM employing a CO-functionalized tip displays dramatically enhanced resolution in imaging covalent bonds of polycyclic aromatic hydrocarbon [18]. Although many STM or Q+AFM images of different classes of molecules within sub-atomic resolution have been generated recently, the functionalizing tips method increases experimental difficulties such as the deposition of molecule or atom for tip decoration on surface may change some properties of the target samples. Therefore, the functionalizing tip has experimental limitations and cannot be generalized to any molecules and materials of interest.

### C. Single Image Super Resolution

Single Image Super Resolution attempts to restore a high-resolution image from a low-resolution observation of the same scene. Due to its ill-posedness nature, single image super-resolution is a well-known challenging problem. Recently, powerful deep learning algorithms, including Super-Resolution Convolutional Neural Network (SRCNN) [19], SRGAN [16], Deep Recursive Residual Network (DRRN) [20], Enhanced Deep Residual Network (EDRN) [21], Deep Back Projection Network (DBRN) [22], and many others, have been developed for Single Image Super Resolution and have achieved attractive results in many applications. Yang et al. [23] provides a thorough survey of the available deep learning architectures for Single Image Super Resolution.

In this work, different from the existing experimental methods for STM and Q+AFM image super-resolution, inspired by the effectiveness of deep learning methods for single image super-resolution, we attempt to use the experiment-generated high-resolution STM and Q+AFM images on a wide variety of molecules to generally enhance low-resolution STM and Q+AFM images. We adopt a deep learning architecture similar to SRGAN to implement STM and Q+AFM image super-resolution.

## III. Methods

### A. STM and AFM Data Collection

We collect 160 high-resolution STM images of a wide variety of molecules available from the public domain to train STM-SR. These STM images are obtained by high-resolution STM experiments with functionalizing tips. Additional 40 experiment-generated, high-resolution STM images, which are on molecules different from those in the training set, are collected and used as the test set to evaluate the performance of STM-SR. Under the similar principle, 152 high-resolution Q+AFM images are used to train AFM-SR and 37 are set aside as test set for AFM-SR. All of these high-resolution STM and Q+AFM images are scaled to 256x256. Data augmentation methods, such as rotation, and vertical and horizontal reflections, are applied to increase the size of training samples.

### B. Deep Learning Architectures of STM-SR and AFM-SR

Both STM-SR and AFM-SR programs adopt the similar mechanism as that of SRGAN. As a Generative Adversarial Network (GAN) architecture [24], STM-SR consists a generator and a discriminator, which are illustrated in Figure 1. AFM-SR shares the same deep learning architecture as STM-SR, except for being trained using high-resolution AFM images. Here we only illustrate the architecture of STM-SR.

In the STM-SR generator, the low-resolution STM image is fed as input through a convolutional layer of 9x9 kernels and 64 feature maps followed by a Parametric ReLU layer. The next layers utilize 16 residual blocks, each including a convolutional layer of 3x3 kernels and 64 feature maps followed by a batch normalization layer, a Parametric ReLU activation function, another convolutional layer with batch normalization, and a final elementwise sum method by adding up the feedforward output with the skip connection output [25]. Then the upsampling block, consisting of a convolutional layer, a upsampling layer, and a leaky ReLU activation, is used to resize toward the size of the target high-resolution STM image. The rest of the generator model is constructed by 2 upsampling blocks, a convolutional layer, and a Sigmoid activation function to generate the high-resolution STM image. In STM-SR, the input low-resolution STM images are 64x64 monotone images and the output is 256x256 high-resolution images.

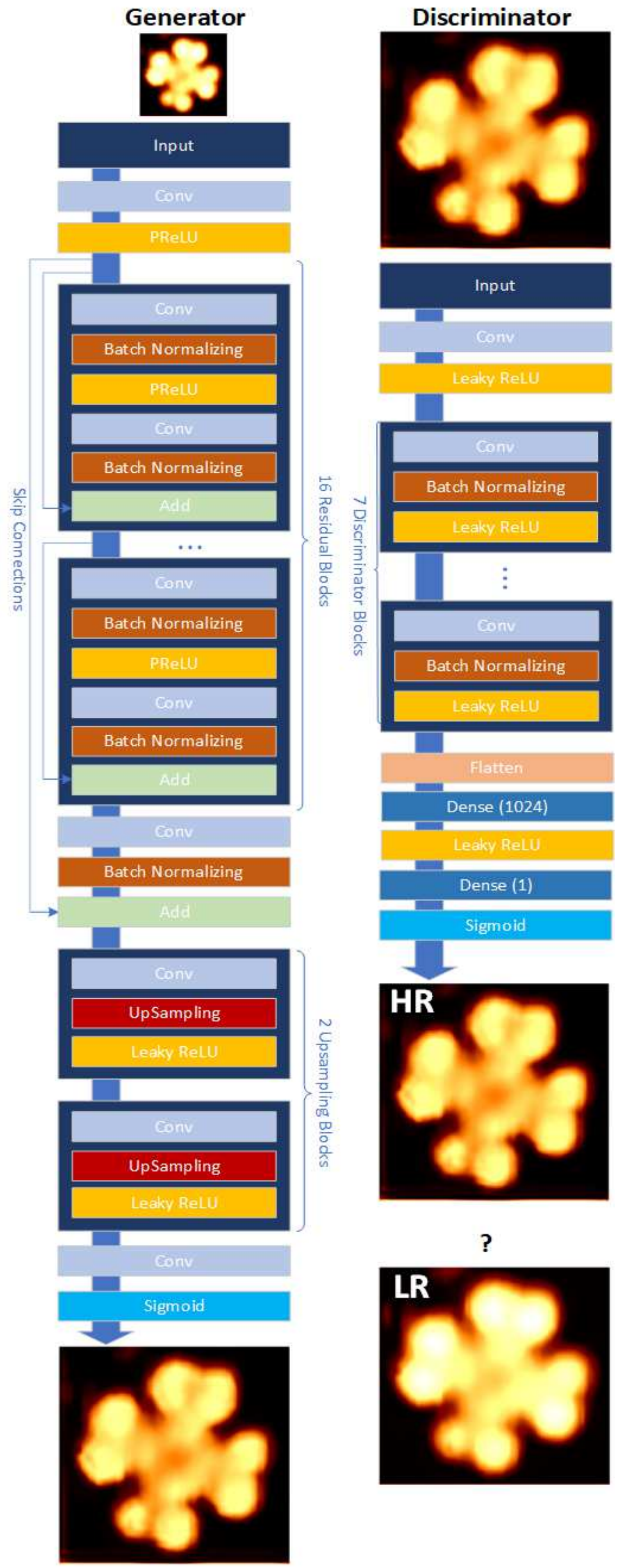


Figure 1: Architectures of the Generator and Discriminator in STM-SR

The STM-SR discriminator architecture makes use of an initial convolutional layer followed by a Leaky ReLU activation function. Then, after 7 repetitive discriminator blocks, each containing a convolutional layer, a batch normalizing layer, and a Leaky ReLU activation function, a single one-dimensional vector is converted by a flatten layer. Afterwards, a series of fully-connected dense layers followed by a Sigmoid activation function are used to classify the true and the generated fake images. The discriminator helps the generator to effectively learn the features of high-resolution STM images.

Similar to the SRGAN, the overall loss of the STM-SR is the weighted sum of the content loss measured by Visual Geometry Group (VGG) [26] loss and the adversarial loss. This loss allows the STM-SR model to focus on improving the overall quality of the STM image instead of pixel-by-pixel comparison.

## IV. Results

### A. Evaluation Metric

Peak Signal to Noise Ratio (PSNR) is used to measure how similar the reconstructed super-resolution image $O$ is to the actual high-resolution STM image $P$ with sizes of $m \times n$. The mean squared error (MSE) between images $O$ and $P$ is defined as

$$MSE = \frac{1}{mn}\sum_{i=1}^{m}\sum_{j=1}^{n}[O(i,j) - P(i,j)]^2.$$

Then, PSNR is defined as

$$PSNR = 10 \cdot \log_{10}\frac{{MAX_P}^2}{MSE},$$

where $MAX_P$ denotes the maximum signal value that exists in the original high-resolution STM image $P$.

### B. Performance of STM-SR

We use the widely used bicubic interpolation method [27] as the baseline to compare with the deep learning-based super-resolution methods on converting low-resolution STM images (64x64) to high-resolution ones (256x256). Figure 2 shows the super-resolution results of bicubic interpolation and STM-SR on three STM images in the test set as examples. One can find that STM-SR yields a significantly higher PSNR than bicubic interpolation, while visually reconstructing the high-resolution STM images and generating more structural details. On the overall test set with 40 STM images, the mean PSNR of bicubic interpolation is 17.02 with standard deviation of 6.02. In comparison, the mean PSNR of STM-SR is 27.35 with standard deviation of 5.51.

It is also interesting to note that STM-SR can even fix the flaws in the experimental STM images. The experimental image in Figure 2(b) shows a scratch throughout the image. This is typically generated by the STM tip from disruptions in tunneling current oscilations. These tunneling current oscilations can be affected by noise and minor interactions with the surface during scanning. Nevertheless, when generating the high-resolution STM images, STM-SR is able to reconstruct the atoms that are striked through by the scratch in the original high-resolution STM image.

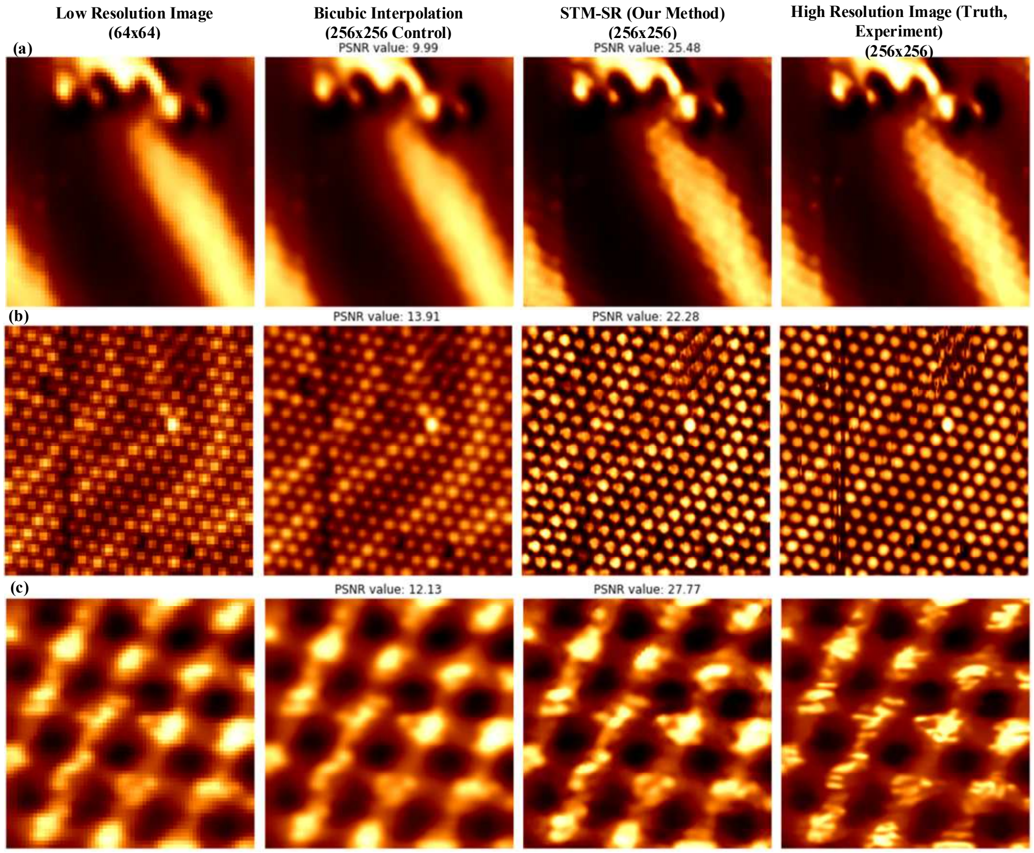


Figure 2: Comparison of results on three STM samples in the test set

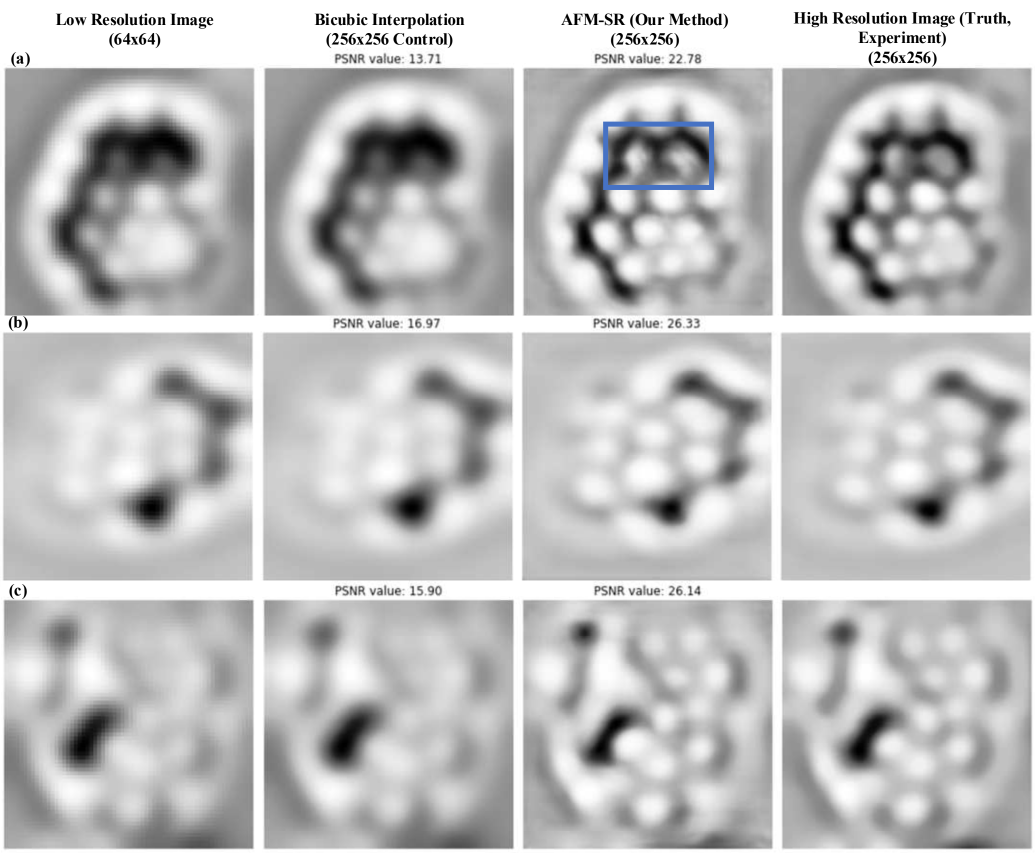


Figure 3: Comparison of results on three Q+AFM samples in the test set

### C. *Performance of AFM-SR*

Similar to the results of STM-SR, Figure 3 shows that AFM-SR is able to generate sharper high-resolution Q+AFM images with more details than bicubic interpolation. AFM-SR generates high-resolution images with better PSNR. On the overall test set with 37 Q+AFM images, the mean PSNR of bicubic interpolation is 14.62 with standard deviation of 3.20, while the mean PSNR of AFM-SR is 28.11 with standard deviation of 2.50. However, the test case shown in Figure 3(a) indicates that AFM-SR has the potential to generate unphysical artifacts. The two atoms highlighted in the blue box in the high-resolution Q+AFM image generated by AFM-SR are over-constructed with unphysical patterns. Finding the cause of these unwanted artifacts and removing them will be our future research work.

## V. CONCLUSION

In this study, we develop and apply deep learning-based super-resolution techniques to break the experimental resolution limits of STMs and Q+AFMs. We train STM-SR and AFM-SR models adopting the SRGAN architecture to convert the low-resolution images into high-resolution ones. Our results demonstrate that STM-SR and AFM-SR are able to generate high quality images that are superior to those generated by conventional bicubic interpolation methods.

## VI. FUTURE WORK

Our results show that the deep learning models for STM and Q+AFM super resolution may generate unphysical artifacts. Our next step will be developing methods to detect and eliminate these unwanted artifacts. Our research direction will be incorporating physics models into the machine learning models.The study presented here is based on the deep learning techniques of “Single Image Super Resolution.” In reality, many images of the same molecule or molecules of the same kind are generated in STM and Q+AFM experiments. Future studies can use “Multiple Images Super Resolution” to piece many molecule images together to form a high resolution one.

Moreover, with the STM and Q+AFM’s ability to generate high-resolution atomic level images outside of its optimal conditions, our research can be extended into many physics and chemistry fields, such as studying sophisticated molecules like prions and other proteins.

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