

A High-Throughput Technique for Color Center Quantification with Neural Networks and its Practical Application in a Surface Passivation Study

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1) MOTIVATION:

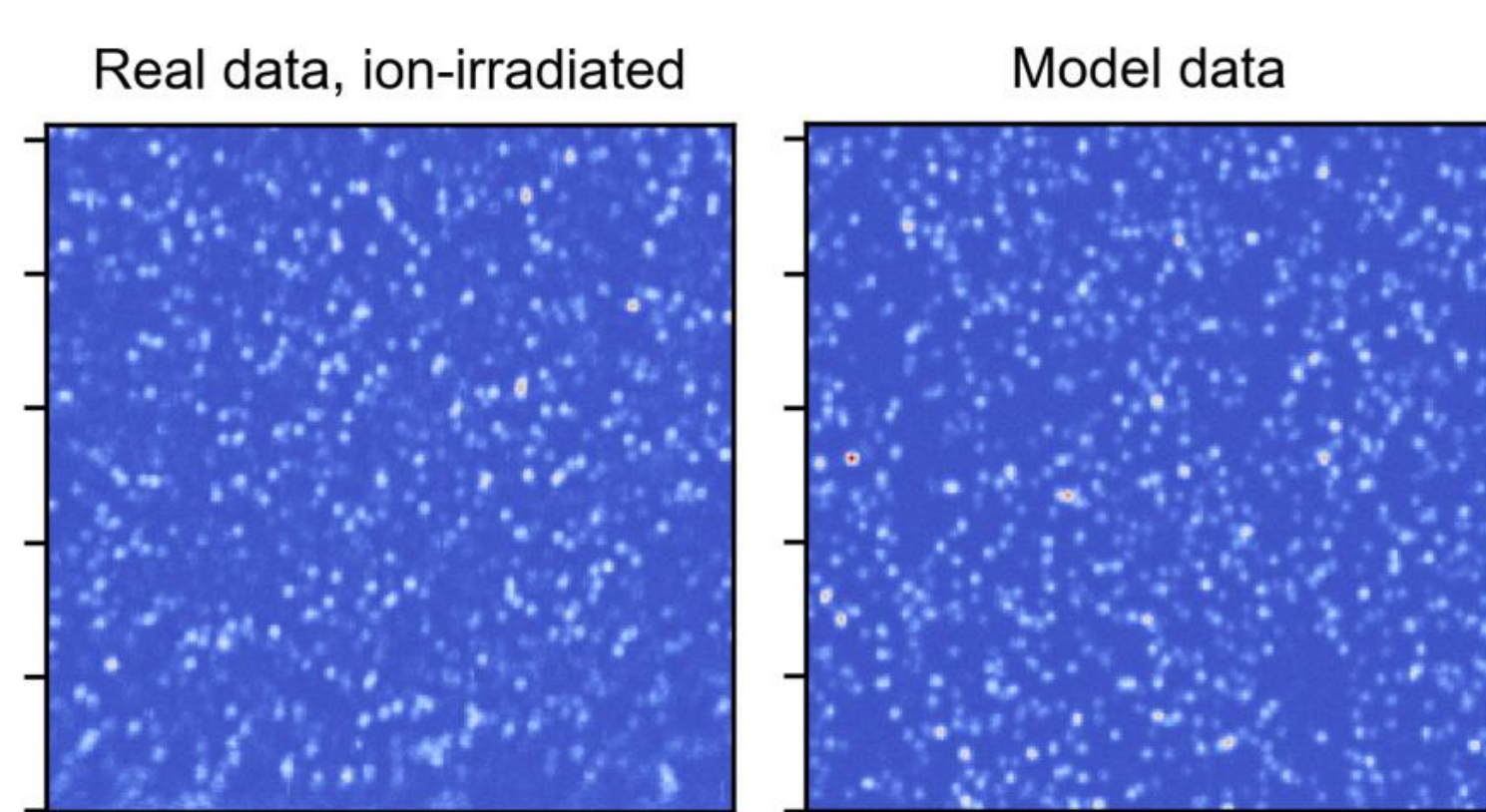
- Technology process and material development for quantum technology devices on 4H-SiC **requires monitoring of color center generation yields.**
- State-of-the-art method employing $g^{(2)}$ autocorrelation measurements¹ not feasible for in-line monitoring due to
 - excessive time consumption
 - required nanofabrication tools (special focused ion beam² or electron beam lithography³)
- $V_{Si}(h)$ color centers (V1) in 4H-SiC have a characteristic photoluminescence (PL) brightness at room temperature⁴
- Goal:** High-throughput, fast-feedback method for the measurement of color center generation yields **compatible with in-line process development**, skipping nanofabrication and subsequent $g^{(2)}$ measurements

2) METHODS:

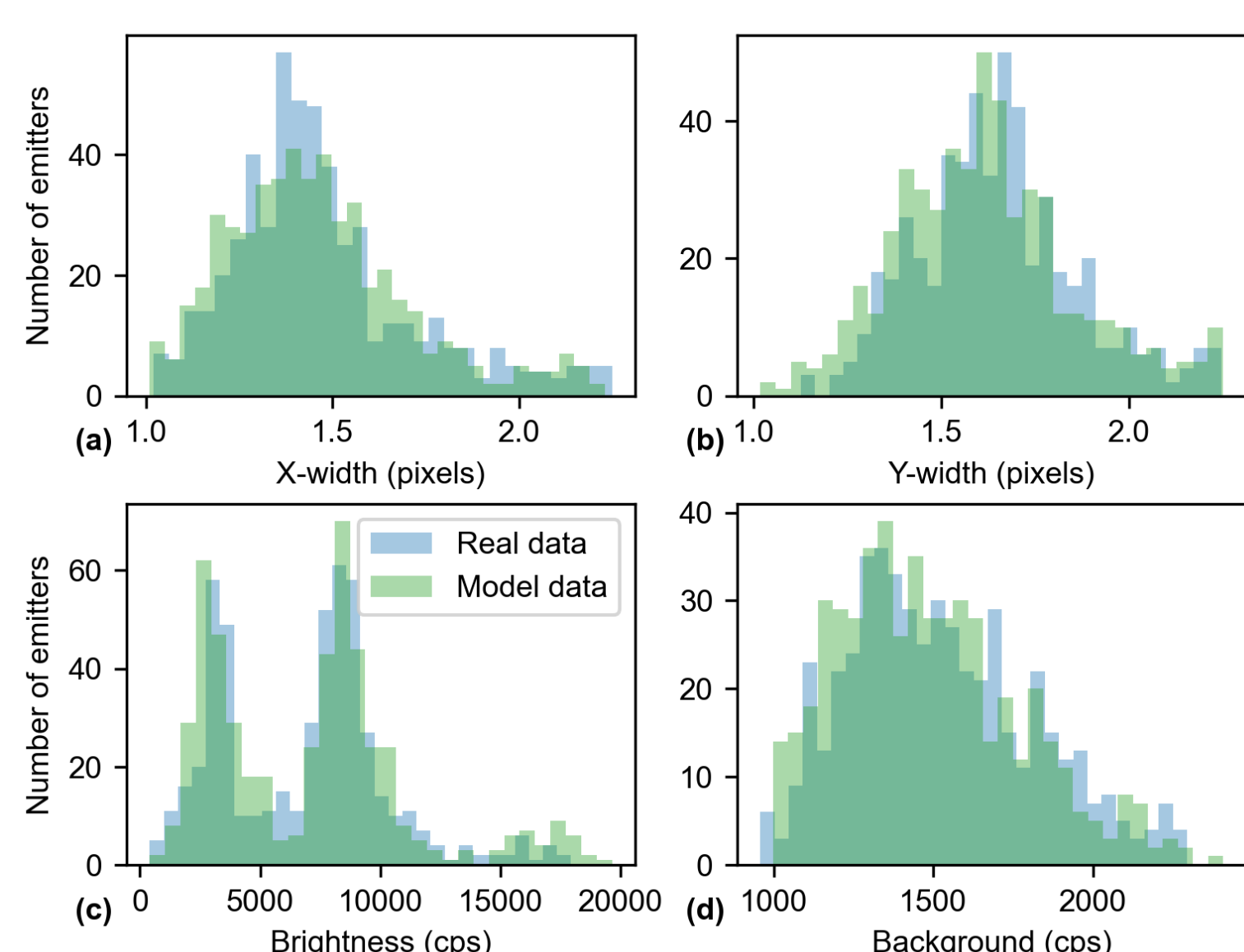
- Sample fabrication:
 - Commercial 4H-SiC substrates, growth of 10 μm homoepitaxial layer, nominally undoped, diced into 5 $\times$ 5 mm^2 coupons
 - V_{Si} color center fabrication by 10 keV He^+ ion irradiation, full area, dose variation $3.3 \times 10^8 \text{cm}^{-2}$ - $9.6 \times 10^8 \text{cm}^{-2}$
 - Post-irradiation thermal anneal: 600 °C, 30 minutes, in vacuum
- Convolutional neural network for deconvolution of RT PL mappings
 - Generation of accurate model data for network training
 - Pre- and post-processing of input data
- Photoluminescence mapping $\sim 32 \times 32 \mu\text{m}^2$, 256 $\times$ 256 pixels
 - Room temperature (RT) for neural network input images, 1 hour per mapping
 - 5 K mapping and photoluminescence spectroscopic investigation for calibration
- Fully automatic statistical evaluation of color center quantification and generation yield determination with proper uncertainty calculations

3) RESULTS

3.1) Training Data Generation



Left: Real confocal PL mapping data of a He ion-irradiated 4H-SiC sample.
Right: Corresponding synthetic model data generated with the calibrated model data generator.

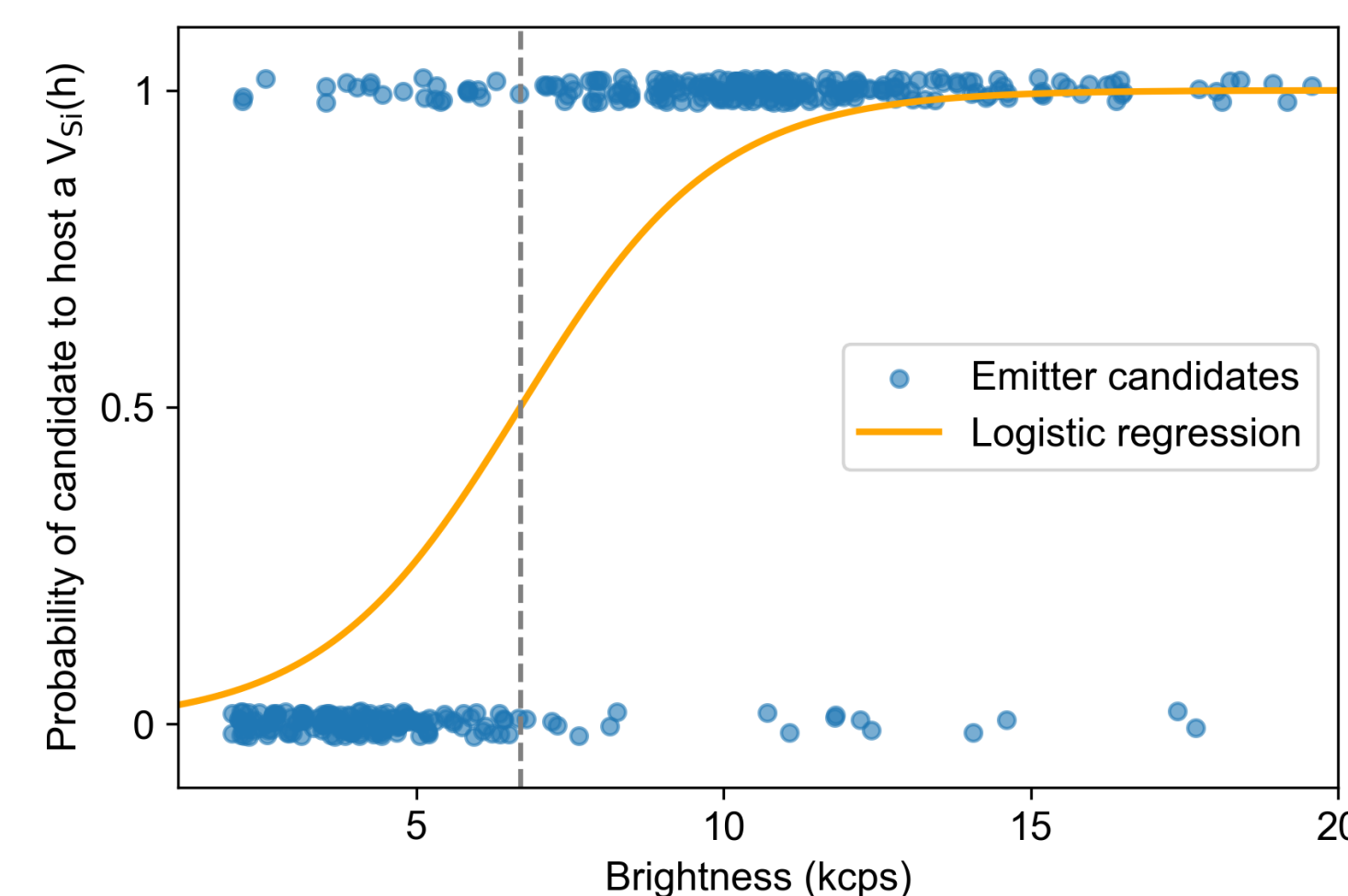


Parametrization of emitter characteristics⁴ for real and synthetic PL mapping data, respectively:

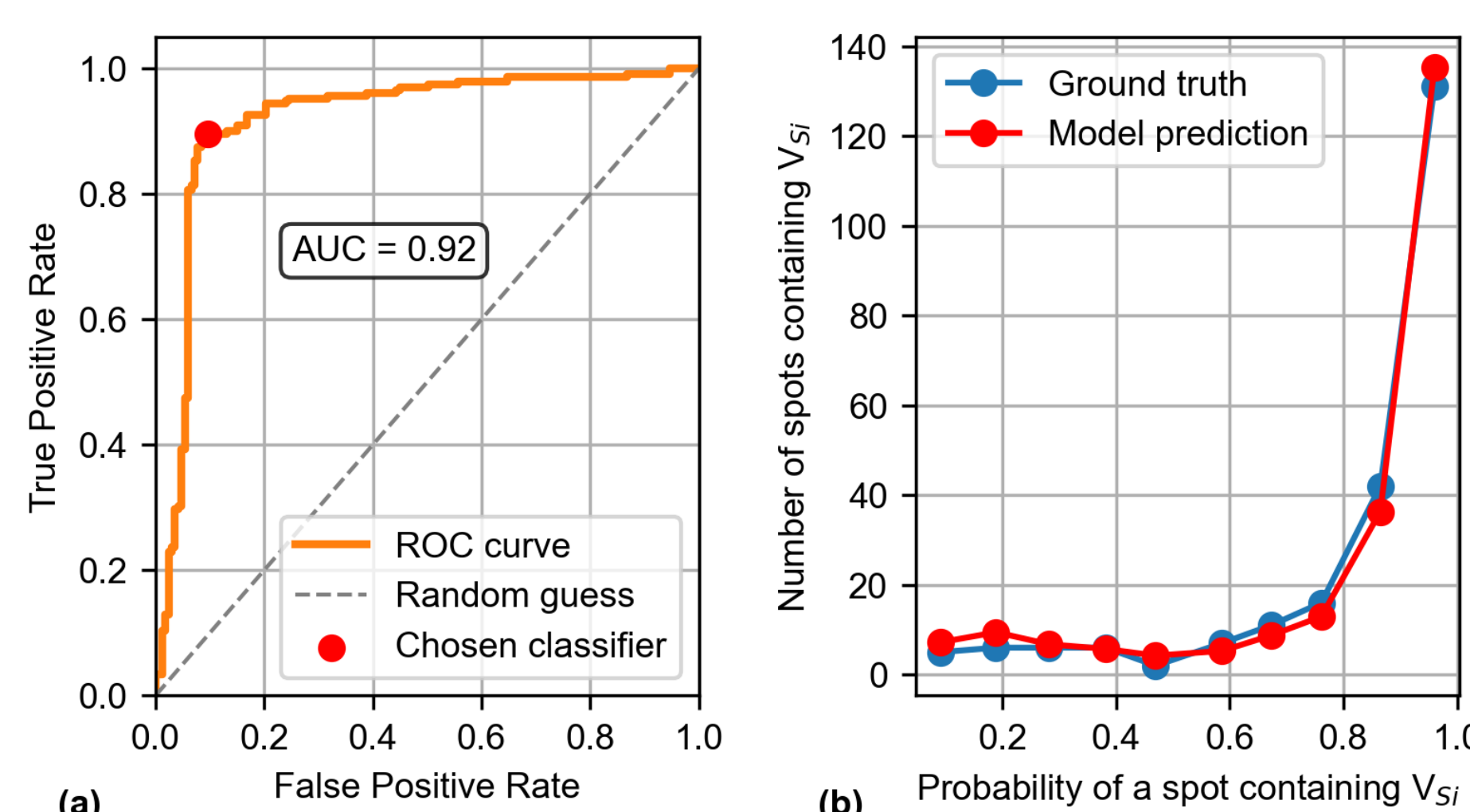
- (a)-(b): Width parameter of the point spread function
 (c): Emitter brightness distribution
 (d): Emitter background distribution

- Generated synthetic data for network training shows identical parameters as real data

3.2) Correlation of Room Temperature PL Emitter Brightness and Emitter Type



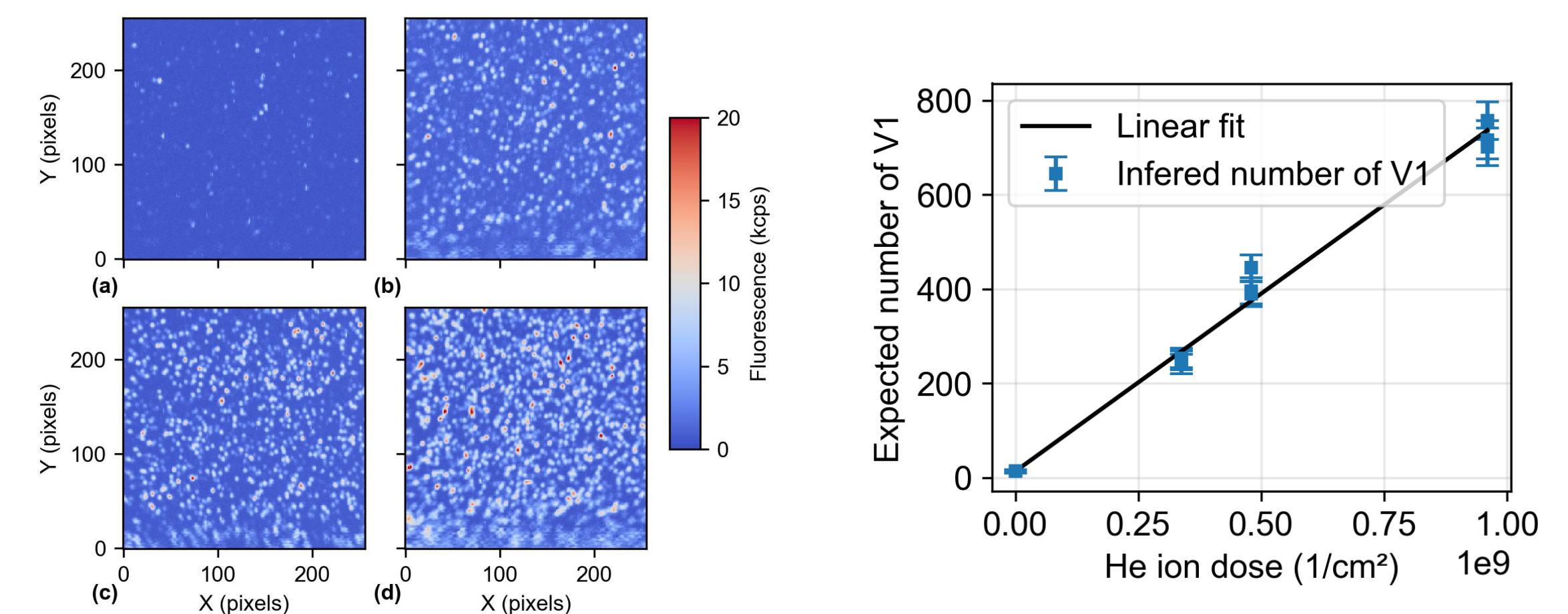
Logistic regression of 400 spectroscopically classified emitters vs. their room temperature PL brightness values. The fit function provides a brightness-dependent measure for the probability of an emitter candidate to contain a V1 color center.



- (a): Receiver operating characteristic (ROC) for the classification of the emitter type by emitter brightness.
 (b): Reliability plot for the fitted logistic regression function above.

- Strong classification of emitter type (V1 or not V1) by emitter brightness with a reliable probability model
- Accuracy, precision and recall for V1 around 90 %

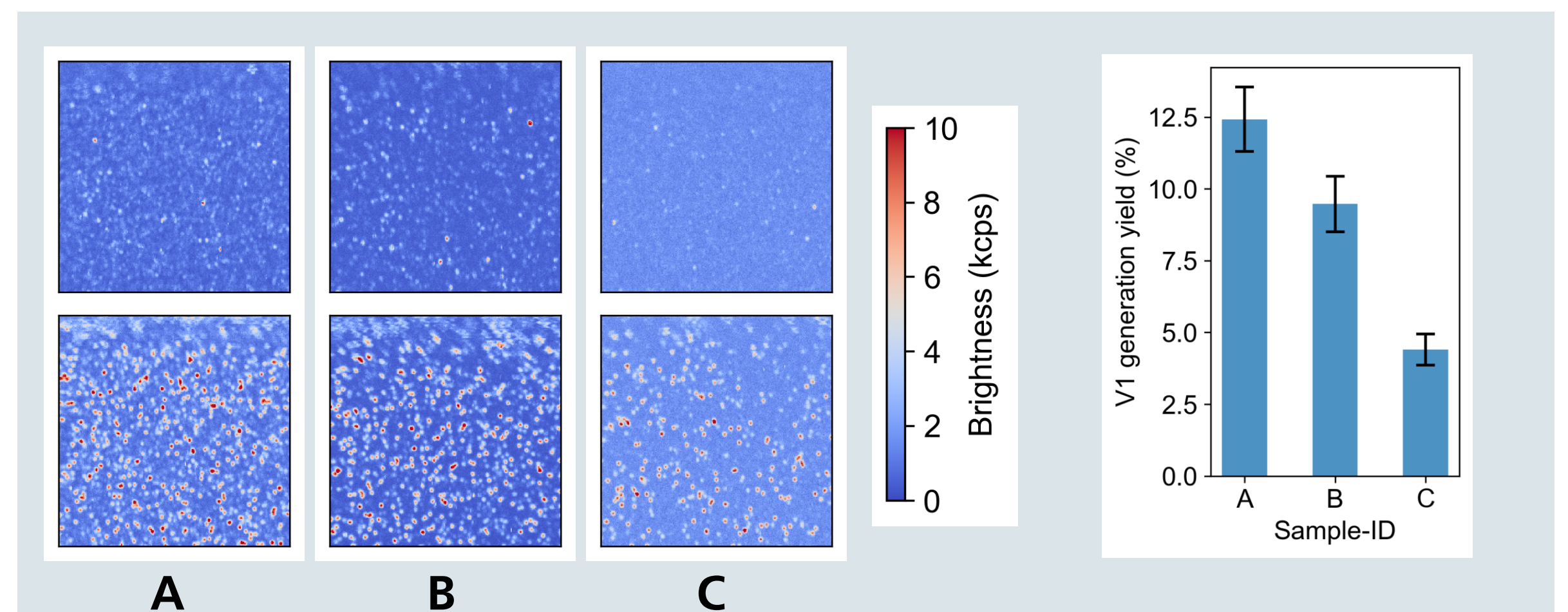
3.3) Application to a Benchmark Sample Set and Surface Passivation Study



PL mappings of benchmark samples:

- (a): non-irradiated
 (b)-(d): irradiated with increasing He ion dose.

Number of V1 color centers quantified on the benchmark sample scans by the novel classification approach.



Application of the classification method within a surface passivation study on 4H-SiC samples: Different passivations (A,B,C) result in significantly different V1 color center generation yields. Upper row of scans: Non-irradiated passivated samples. Lower row of scans: He ion-irradiated passivated samples, respectively.

- Color center generation yield can be quantified within 2 hours per sample with the new approach.
- Benchmark samples with He ion dose variation:
 - reveal expected linear irradiation dose dependence
- Fast yield evaluation demonstrated in a large passivation study

4) CONCLUSION AND OUTLOOK:

- Our technique accelerates quantification of color centers and their generation yield, relying completely on room temperature PL mappings
 - Outperforms** state-of-the-art approach with $g^{(2)}$ measurements **by a factor of 50 times in measurement speed with comparable precision**
 - After model calibration, **no need anymore for advanced nano structuring techniques, time-tagging hardware and $g^{(2)}$ measurements**
- Next steps: Exploring method feasibility for other color centers in 4H-SiC as well as in other host materials

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