

Electronic Supplementary Information for the manuscript:

Quantifying Patterns in Optical Micrographs of One- and Two-Dimensional Ellipsoidal Particle Assemblies

Veronica Grebe, Mingzhu Liu and Marcus Weck*

Molecular Design Institute and Department of Chemistry, New York University, New York, NY 10003, USA

Supplementary Figures

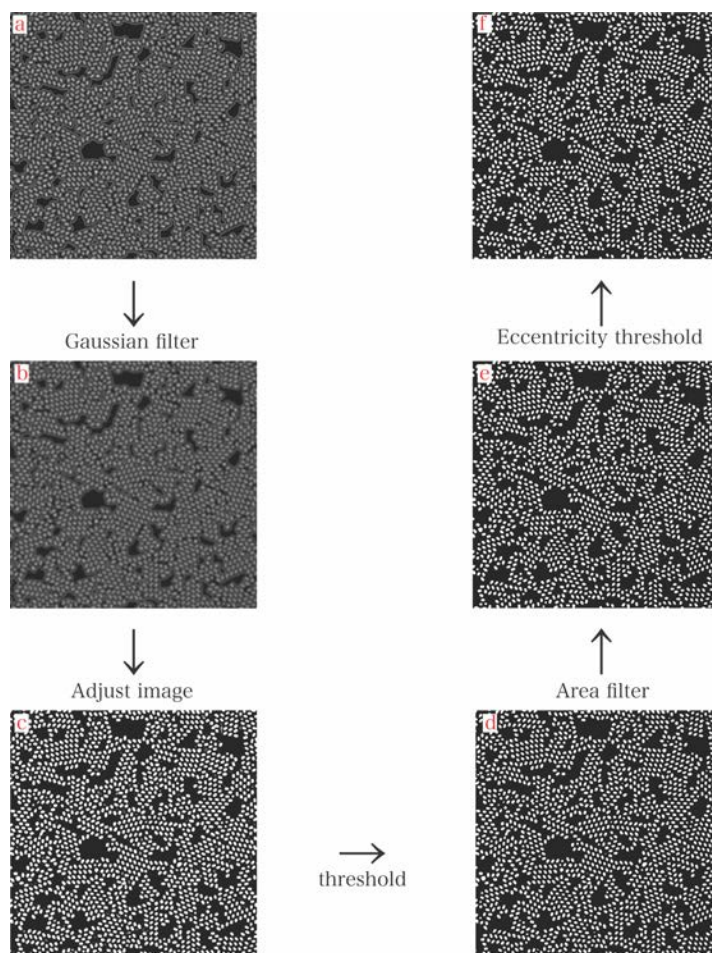


Figure S1. Typical image segmentation. (a) The particles are first removed from the background by filtering based on local standard deviation. (b) The holes created in the particle centers are blurred and removed by applying a Gaussian filter. (c) The particle features are then made brighter by adjusting the image intensity values, which allows for a threshold (d) to be applied to create a binary image and fully separate the particle from the background. The image features that are not of interest are then removed by filtering out features both above and below defined thresholds for area (e) and eccentricity (f).

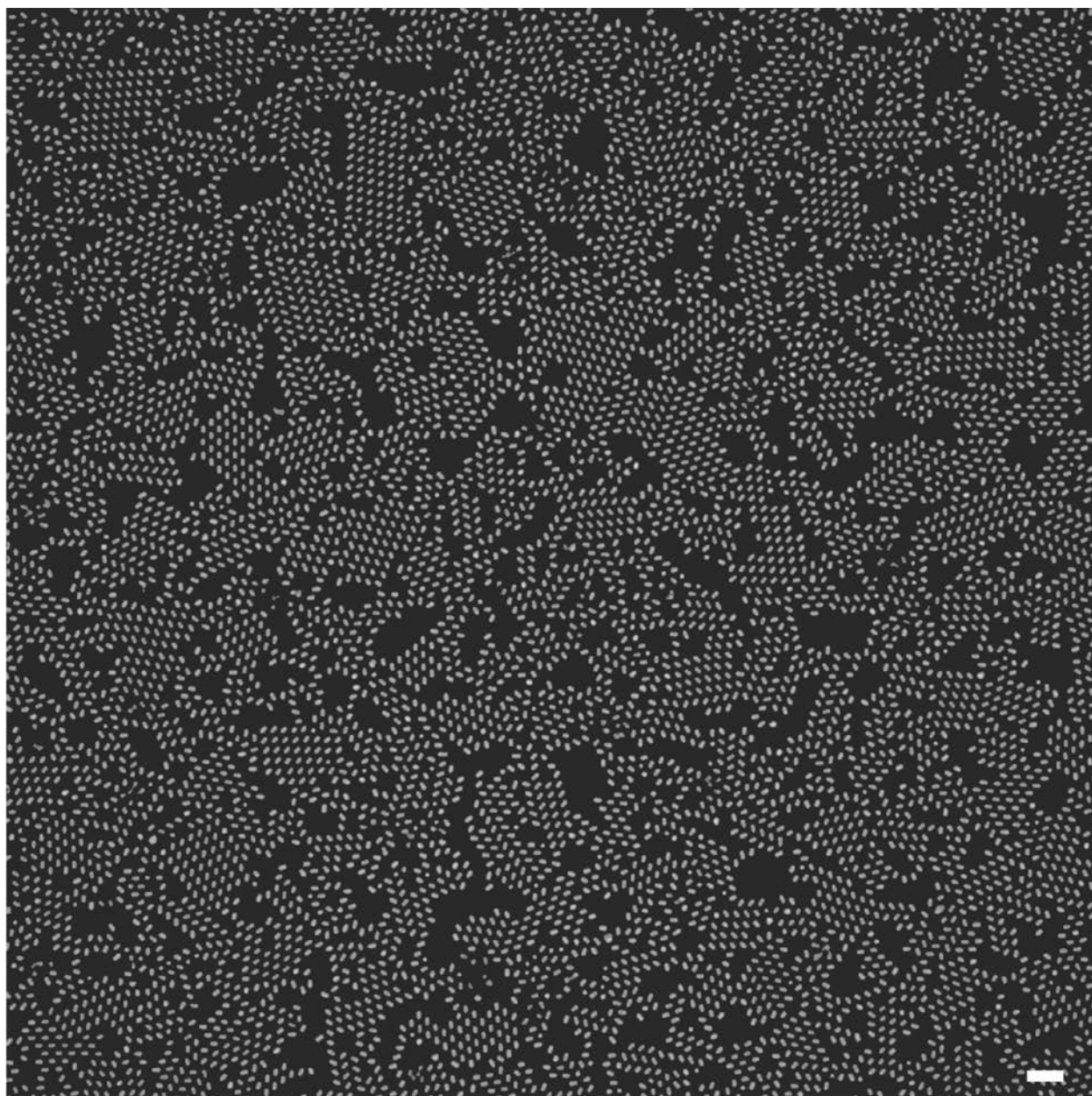


Figure S2. Background masking for particle segmentation. The original image is masked, where black pixels represent the background. The particles that are recognized by the algorithm remain. Scale bar, 5 μm .

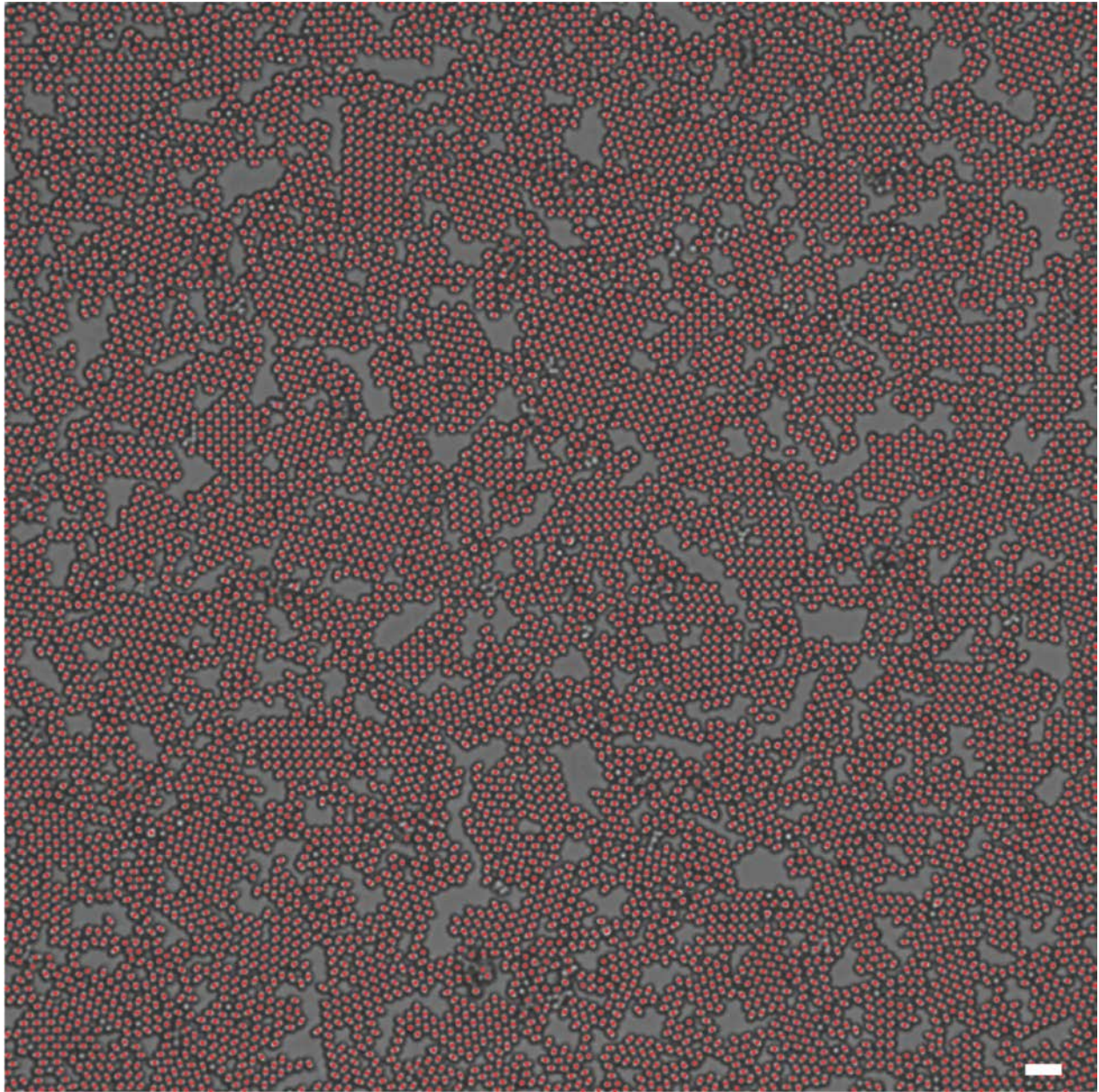


Figure S3. Locating particle centers. The centers of the located particles are shown in red. In this image, 8276 particles are located. Scale bar, 5 μm .

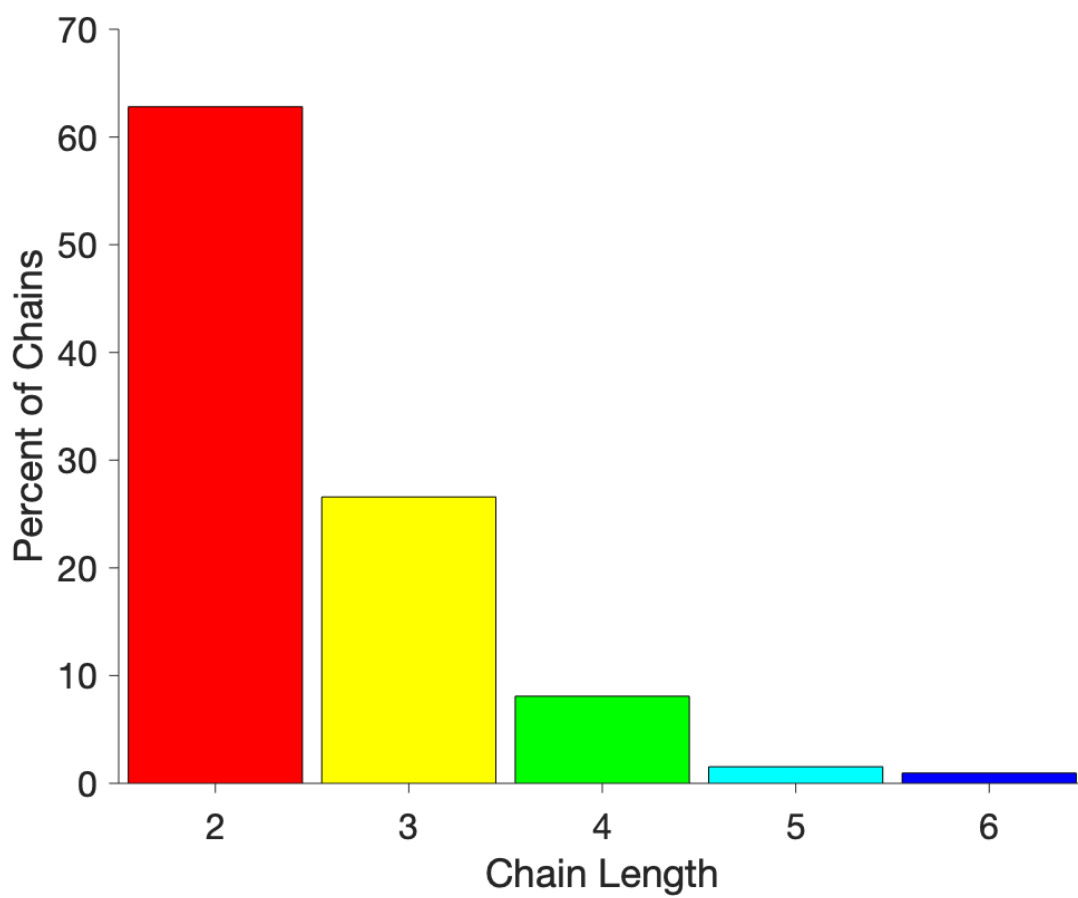


Figure S4. Percent of chains as a function of chain length. The percent of particles that constitute chains is shown as a function of chain length, where the particles constituting no chains (singular particles) are removed from the overall count.

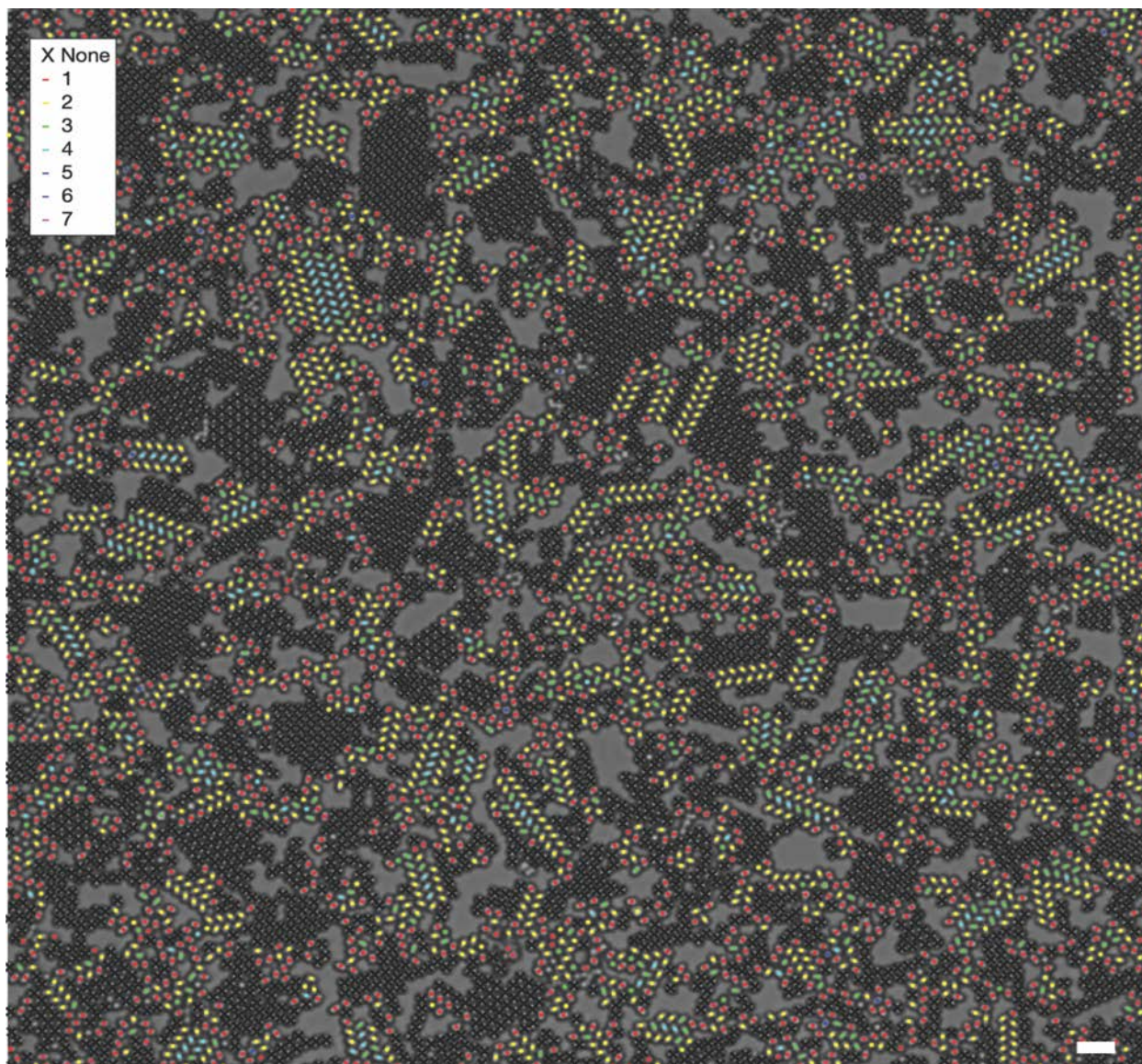


Figure S5. Labeled neighbor count of perpendicular neighbors of the *cmm* vs. *pgg* image. The number of neighbors that have a perpendicular relationship with the center particle are color labeled. This intermediate figure is generated to aid in the creation of the classification rules. Scale bar, 5 μm .

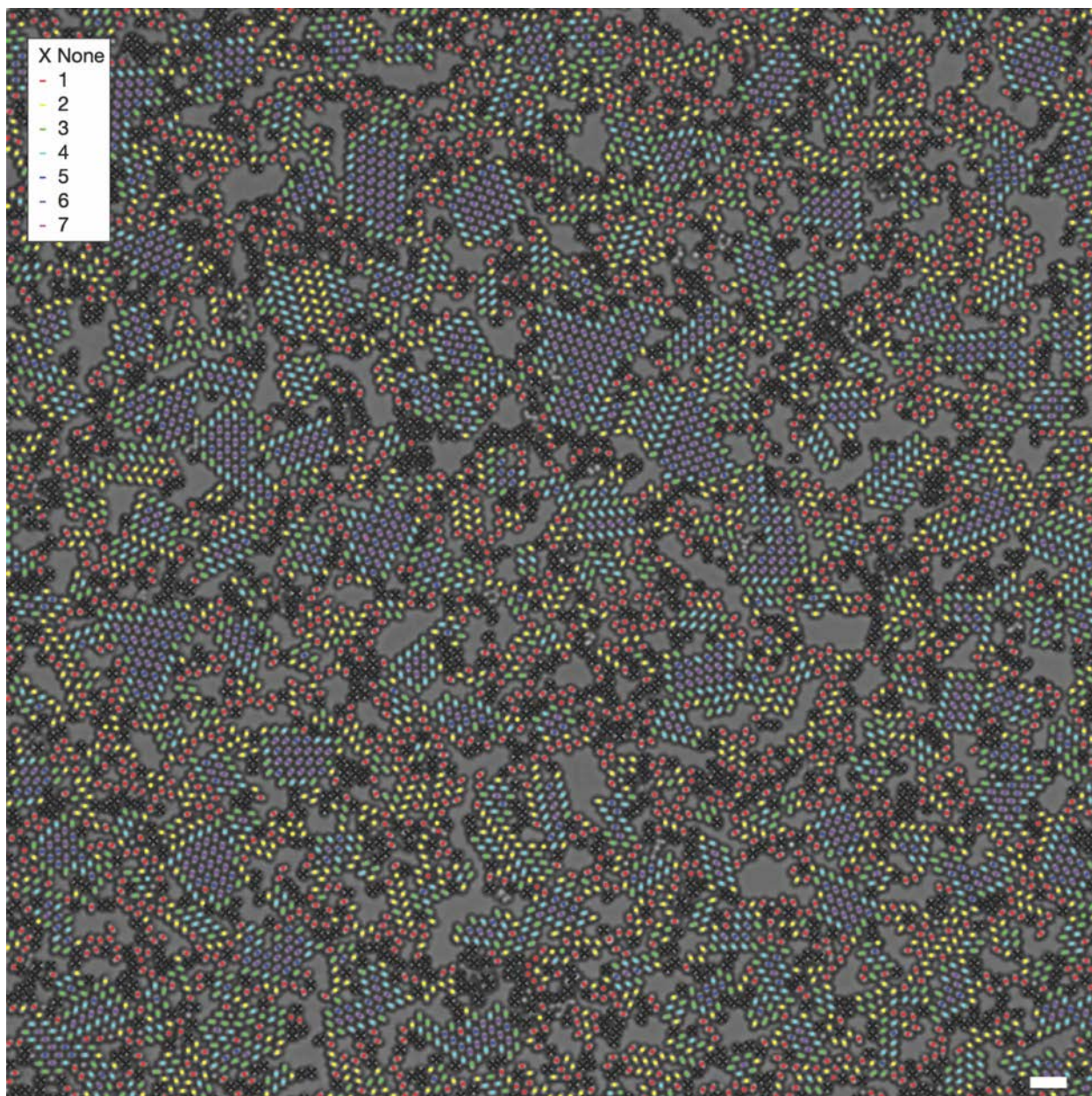


Figure S6. Labeled neighbor count of parallel neighbors of the *cmm* vs. *pgg* image. The number of neighbors that have a parallel relationship with the center particle are color labeled. This intermediate figure is generated to aid in the creation of the classification rules. Scale bar, 5 μm .

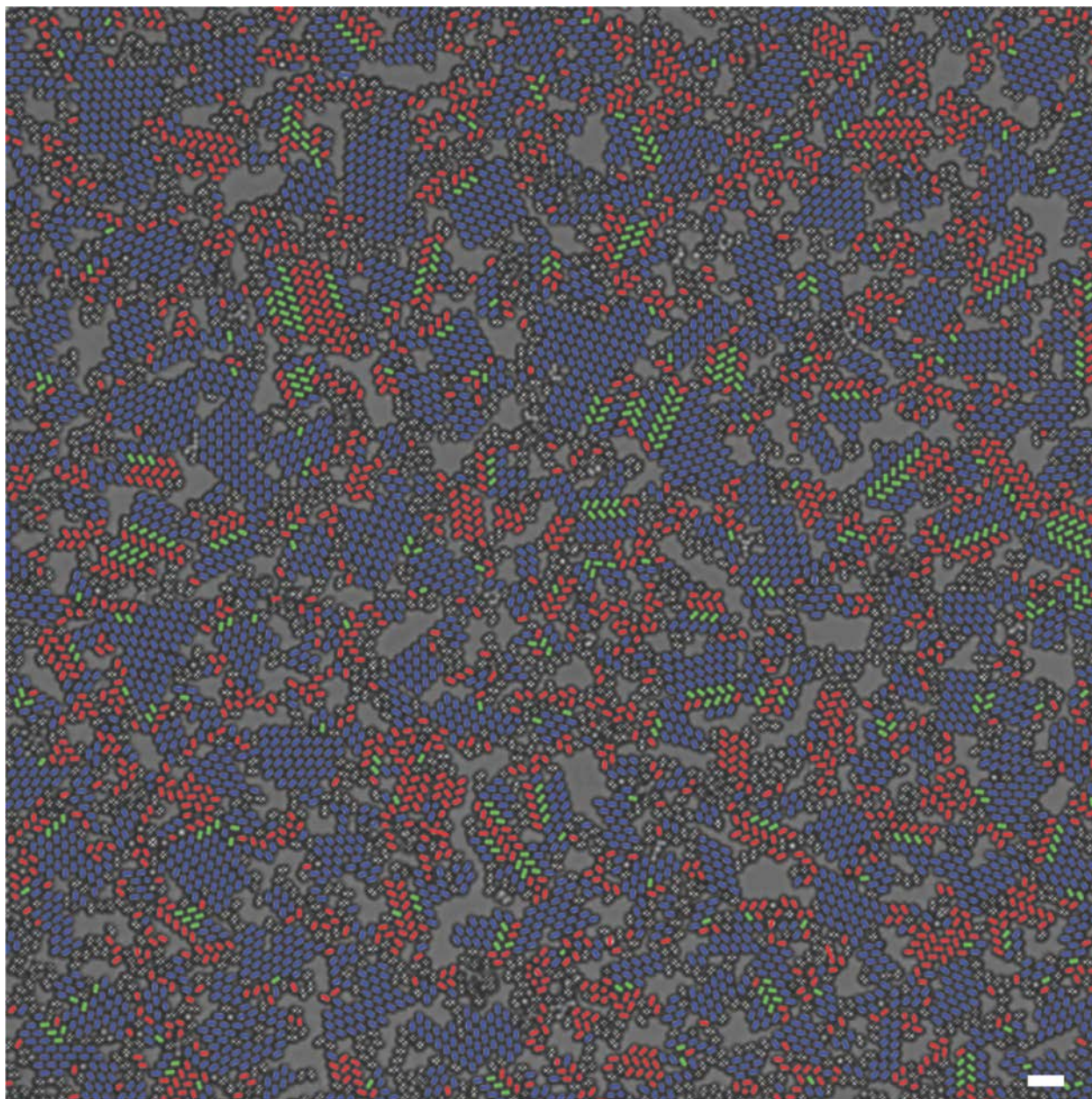


Figure S7. Labeled initial particle classification of the *cmm* vs. *pgg* image. The particles are classified initially based on the defined classification rules. The initial labels describe particle classes *pgg* (red), boundary (green), or *cmm* (blue), and are outlined based on location within the region. The initial rules notably create overcounting error where the parallel and perpendicular relationships that structured particles have with disordered particles are counted toward the overall neighbor count per rule. Further corrections can be made in the modifying requirements section. Scale bar, 5 μm .

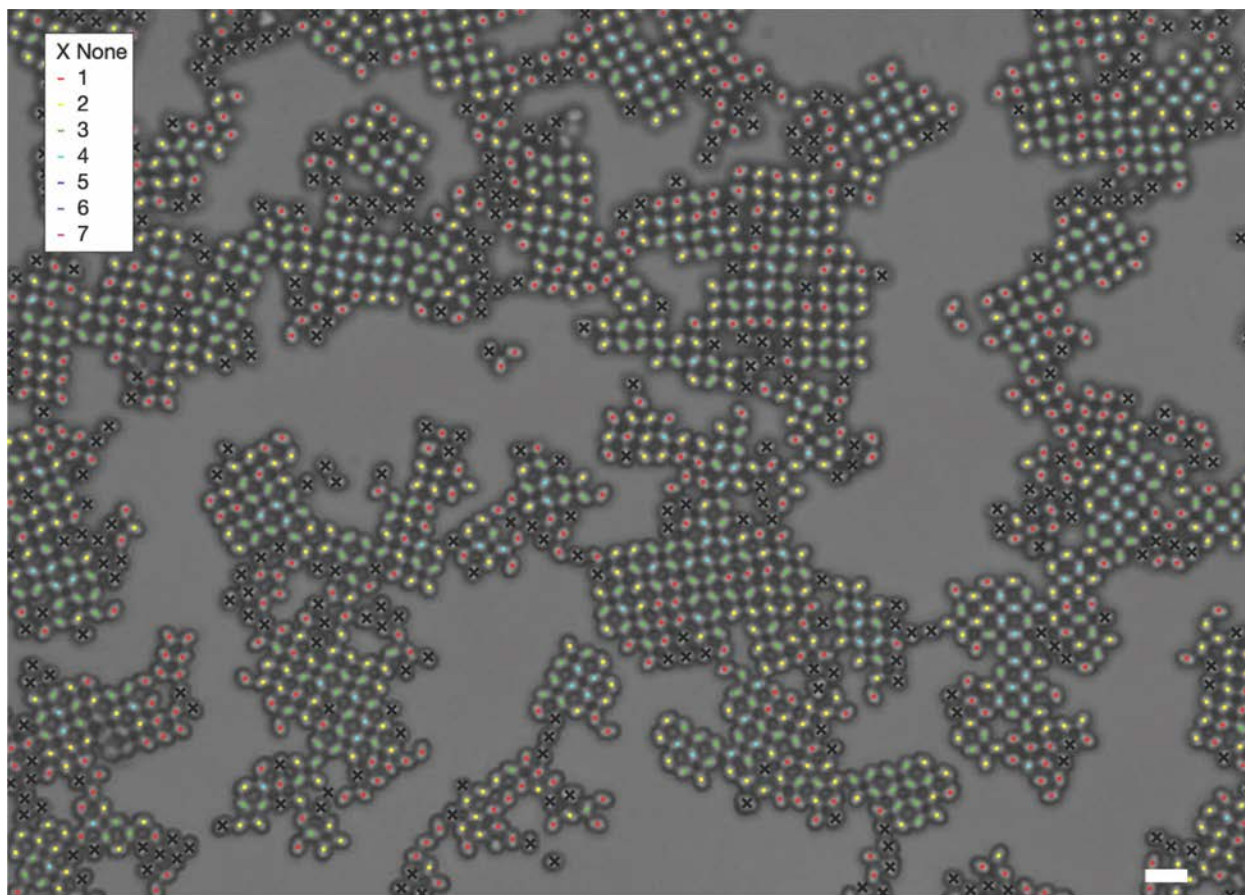


Figure S8. Labeled neighbor count of perpendicular neighbors of the *cmm* vs. *p4m* image. The number of neighbors that have a perpendicular relationship with the center particle are color labeled. This intermediate figure is generated to aid in the creation of the classification rules. Scale bar, 5 μm.

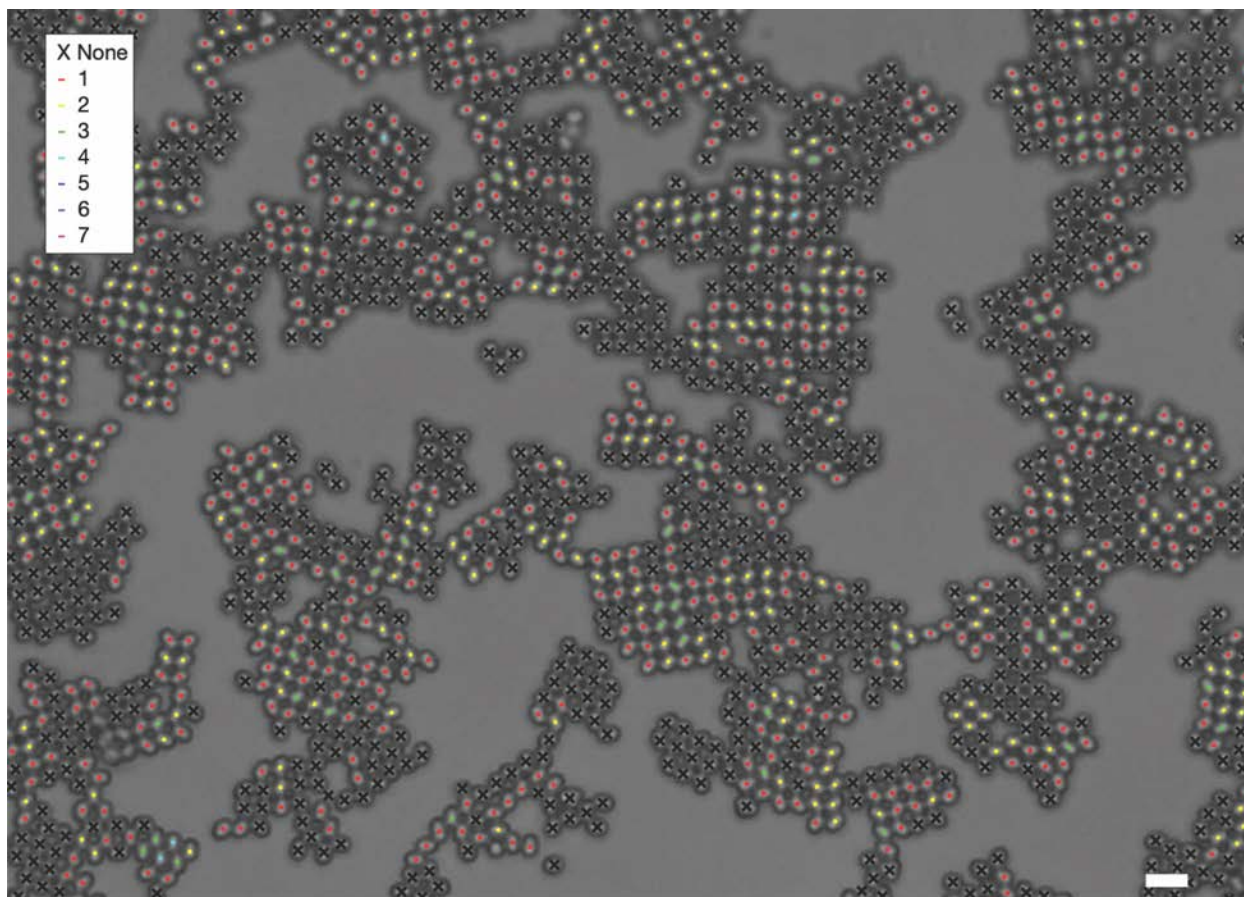


Figure S9. Labeled neighbor count of parallel neighbors of the *cmm* vs. *p4m* image. The number of neighbors that have a parallel relationship with the center particle are color labeled. This intermediate figure is generated to aid in the creation of the classification rules. Scale bar, 5 μm .

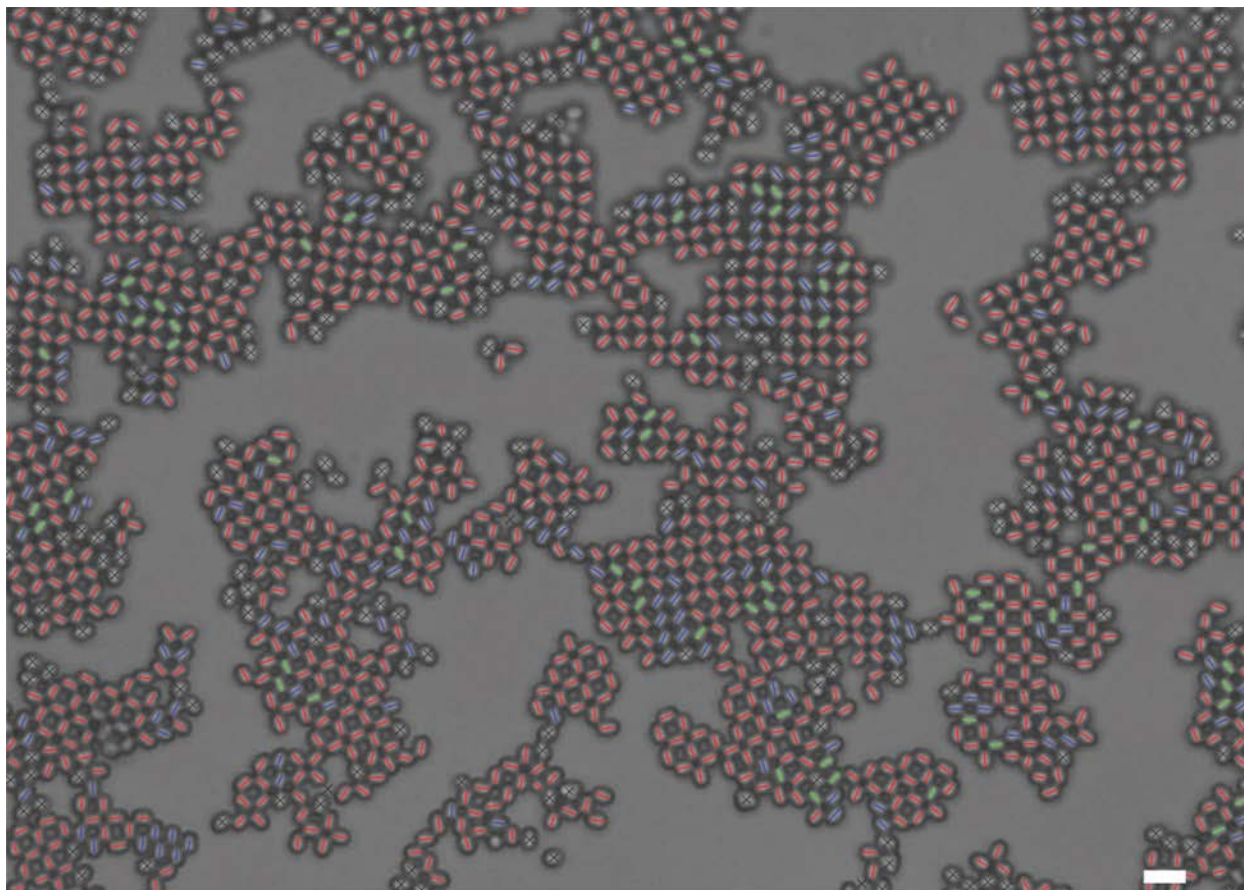


Figure S10. Labeled initial particle classification of *cmm* vs. *p4m* image. The particles are classified initially based on the defined classification rules. The initial labels describe particle classes *p4m* (red), boundary (green), or *cmm* (blue), and are outlined based on location within the region. The initial rules notably create overcounting error where the parallel and perpendicular relationships that structured particles have with disordered particles are counted toward the overall neighbor count per rule. Further corrections can be made in the added requirements section. Scale bar, 5 μm .

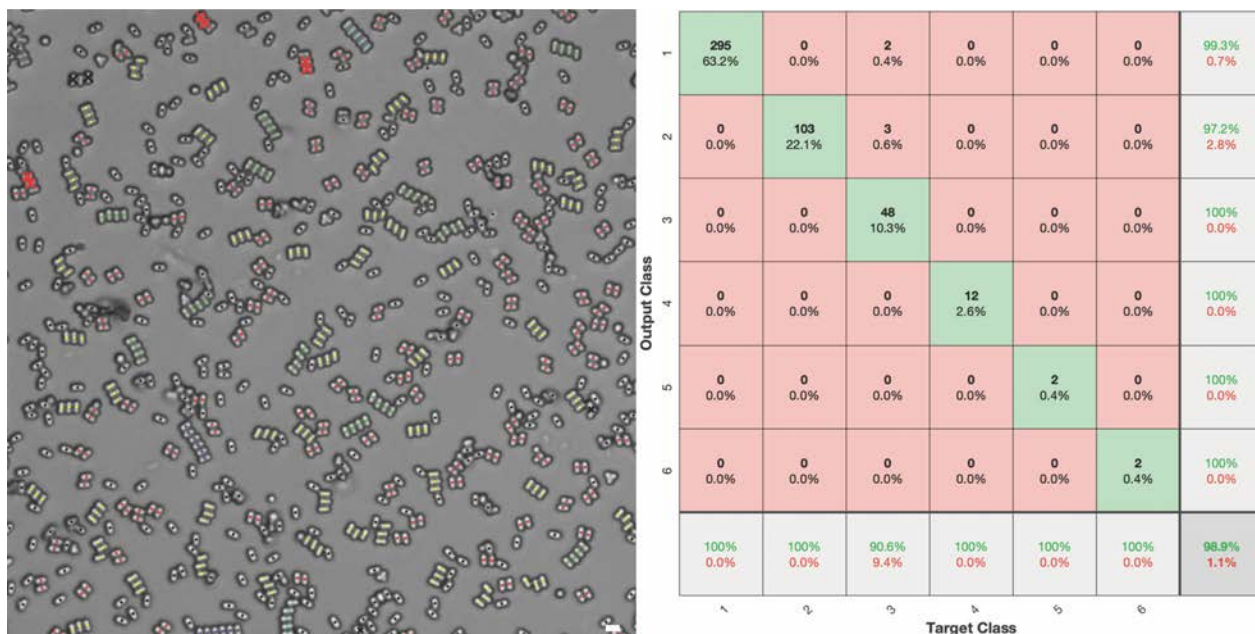


Figure S11. Labeled error of 1D image. The final labels describe particle classes of chain length 1 (black X), 2 (red), 3 (yellow), 4 (green), 5 (light blue), and 6 (dark blue). Correct labels are denoted as dots, where incorrect labels (wrong class) are shown as X. The associated confusion matrix of the 1D image classification error details the algorithm's performance, where the number of chains in each class are considered. The overall accuracy is 98.9%. Scale bar, 5 μ m.

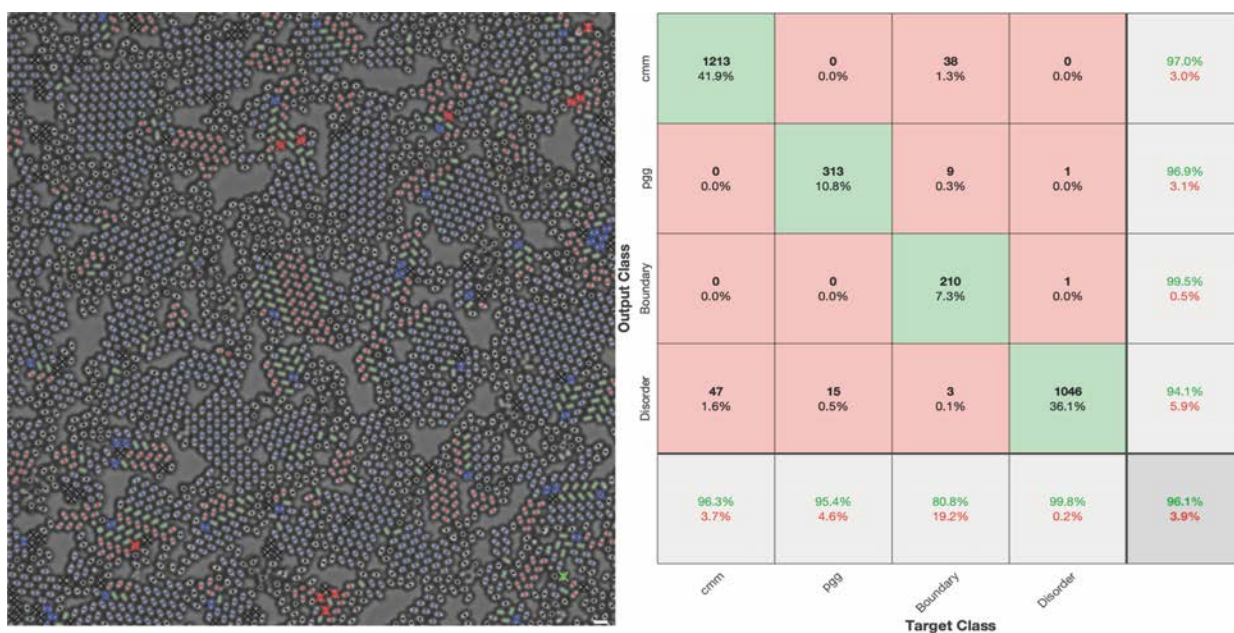
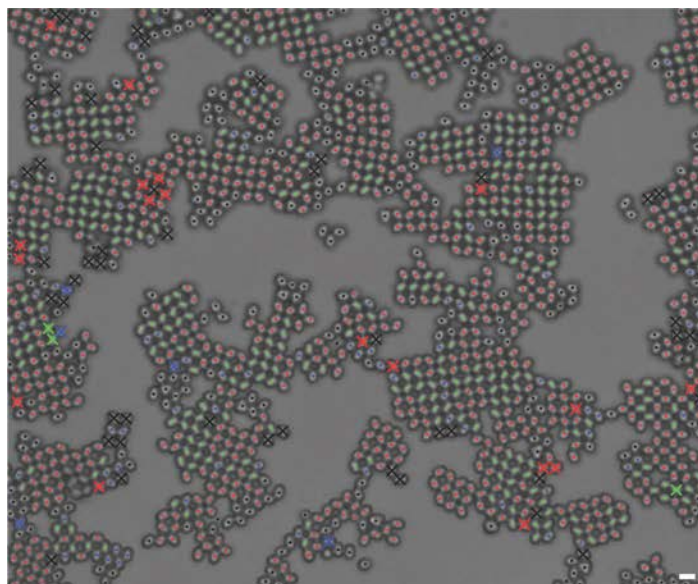


Figure S12. Labeled error of *cmm* vs. *pgg* image. The final labels describe particle classes *pgg* (red), *cmm* (blue), boundary (green), and disordered (black). Correct labels are denoted as dots, where incorrect labels (wrong class) are shown as X. The associated confusion matrix details the *cmm* vs. *pgg* algorithm's classification performance, where the overall accuracy is 96.1%. Scale bar, 5 μ m.



Output Class	<i>cmm</i>	90 6.2%	0 0.0%	2 0.1%	4 0.3%	93.8% 6.2%
	<i>p4m</i>	2 0.1%	706 48.3%	14 1.0%	2 0.1%	97.5% 2.5%
	Boundary	1 0.1%	2 0.1%	307 21.0%	0 0.0%	99.0% 1.0%
	Disorder	31 2.1%	12 0.8%	7 0.5%	261 19.2%	84.9% 15.1%
		72.6% 27.4%	98.1% 1.9%	93.0% 7.0%	97.9% 2.1%	94.7% 5.3%
	<i>cmm</i>	<i>p4m</i>	Boundary	Disorder		
						Target Class

Figure S13. Labeled error of *cmm* vs. *p4m* image. The final labels describe particle classes *p4m* (red), *cmm* (blue), boundary (green), and disordered (black). Correct labels are denoted as dots, where incorrect labels (wrong class) are shown as X. The associated confusion matrix details the *cmm* vs. *p4m* algorithm's classification performance, where the overall accuracy is 94.7%. Scale bar, 5 μm .

Supplementary Tables

<u>Description of each parameter used in the 1D image analysis</u>	<u>Value</u>
Neighborhood used to compute the local standard deviation.	7
Threshold for the calculated standard deviation.	10
Sigma value when applying the Gaussian filter.	1
Lower bound of the range for input intensity when adjusting the image.	50
Upper bound of the range for input intensity when adjusting the image.	150
Lower bound of the range for output intensity when adjusting the image.	0
Upper bound of the range for output intensity when adjusting the image.	255
Threshold for the intensity adjusted image.	205
Lower bound of the range for the area filter.	60
Lower bound of the range for the area filter.	250
Threshold for the eccentricity filter.	0.79
Maximum distance separating particles.	20
Minimum particle major axis length to be counted as in a chain.	7
Minimum particle area to be counted as in a chain.	70
Minimum particle perimeter to be counted as in a chain.	15
Minimum particle-to-particle end-to-center distance to be counted as in a chain.	30
Lower bound of the first angle range of the parallel angle.	-15
Upper bound of the first angle range of the parallel angle.	15
Lower bound of the second angle range of the parallel angle.	165
Upper bound of the second angle range of the parallel angle.	180
The maximum chain length.	6

Table S1. Parameters for 1D optical micrograph analysis. The description and value for each of the input parameters for the analysis of the 1D optical micrograph are described. Each directly correlates with the corresponding MATLAB LiveScript.

<u>Description of each parameter used in the 2D image analysis</u>	<u>cmm</u> <u>vs.</u> <u>p4m</u>	<u>cmm</u> <u>vs.</u> <u>pgg</u>
Neighborhood used to compute the local standard deviation.	11	9
Threshold for the calculated standard deviation.	7	13
Sigma value when applying the Gaussian filter.	3	3
Lower bound of the range for input intensity when adjusting the image.	85	75
Upper bound of the range for input intensity when adjusting the image.	100	100
Lower bound of the range for output intensity when adjusting the image.	0	0
Upper bound of the range for output intensity when adjusting the image.	255	255
Threshold for the intensity adjusted image.	150	190
Lower bound of the range for the area filter.	70	50
Lower bound of the range for the area filter.	400	250
Threshold for the eccentricity filter.	0.2	0.2
Maximum distance separating particles.	23	28
Lower bound of the first angle range of the perpendicular angle.	-110	-120
Upper bound of the first angle range of the perpendicular angle.	-70	-60
Lower bound of the second angle range of the perpendicular angle.	70	60
Upper bound of the second angle range of the perpendicular angle.	110	120
Lower bound of the first angle range of the parallel angle.	-15	-11
Upper bound of the first angle range of the parallel angle.	15	11
Lower bound of the second angle range of the parallel angle.	165	169
Upper bound of the second angle range of the parallel angle.	180	180
Name of the first structure.	cmm	cmm
Lower bound of the number of parallel neighbors for the first structure.	2	2
Upper bound of the number of parallel neighbors for the first structure.	6	6
Lower bound of the number of perpendicular neighbors for the first structure.	0	0
Upper bound of the number of perpendicular neighbors for the first structure.	1	1
Name of the second structure.	p4m	pgg
Lower bound of the number of parallel neighbors for the second structure.	0	1
Upper bound of the number of parallel neighbors for the second structure.	1	2
Lower bound of the number of perpendicular neighbors for the second structure.	1	1
Upper bound of the number of perpendicular neighbors for the second structure.	4	4
Lower bound of the number of parallel neighbors for the boundary particles.	1	2
Upper bound of the number of parallel neighbors for the boundary particles.	4	4
Lower bound of the number of perpendicular neighbors for the boundary particles.	1	1
Upper bound of the number of perpendicular neighbors for the boundary particles.	2	2

Table S2. Parameters for 2D optical micrographs analysis. The description and value for each of the input parameters for the analysis of the 2D optical micrographs are described. Each directly correlates with the corresponding MATLAB LiveScript.