Electronic Supplementary Material (ESI) for Soft Matter.

Hard Superellipse Phases: Particle Shape Anisotropy & Curvature

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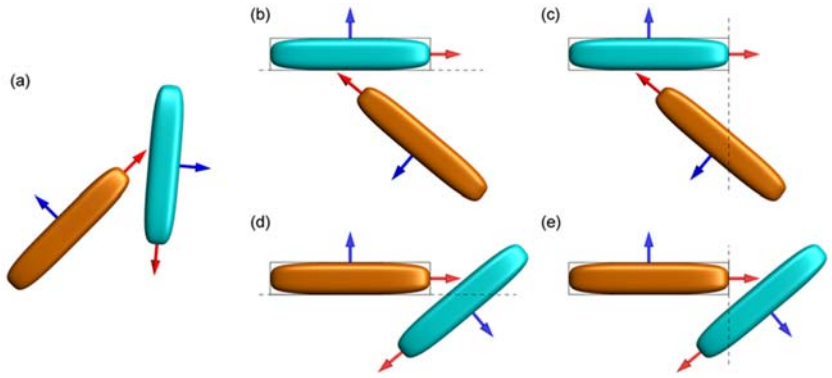

Fig. S1. (a) Schematic of a superellipse pair at a given relative position and orientation. (b-e) Visualization of second approach for overlap condition determined by distance between a plane of a circumscribed rectangle and a second superellipse calculated by Eq. (2). The non-overlap condition is shown in (b).

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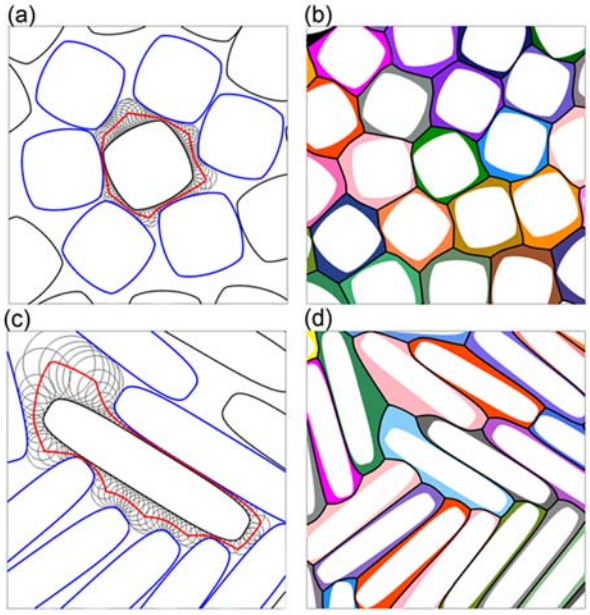


Fig. S2. Visualization of tessellation method to determine superellipse neighbors. For (a) r_y/r_x =1 and n = 1.4, and (c) r_y/r_x =0.2 and n = 4, the tessellation boundary (red) is shown between a central particle (grey) and near neighbors (blue). (b,d) Different colors around each particle (white) show tessellation belonging to each particle.

2. Phase Determination Figures & Tables

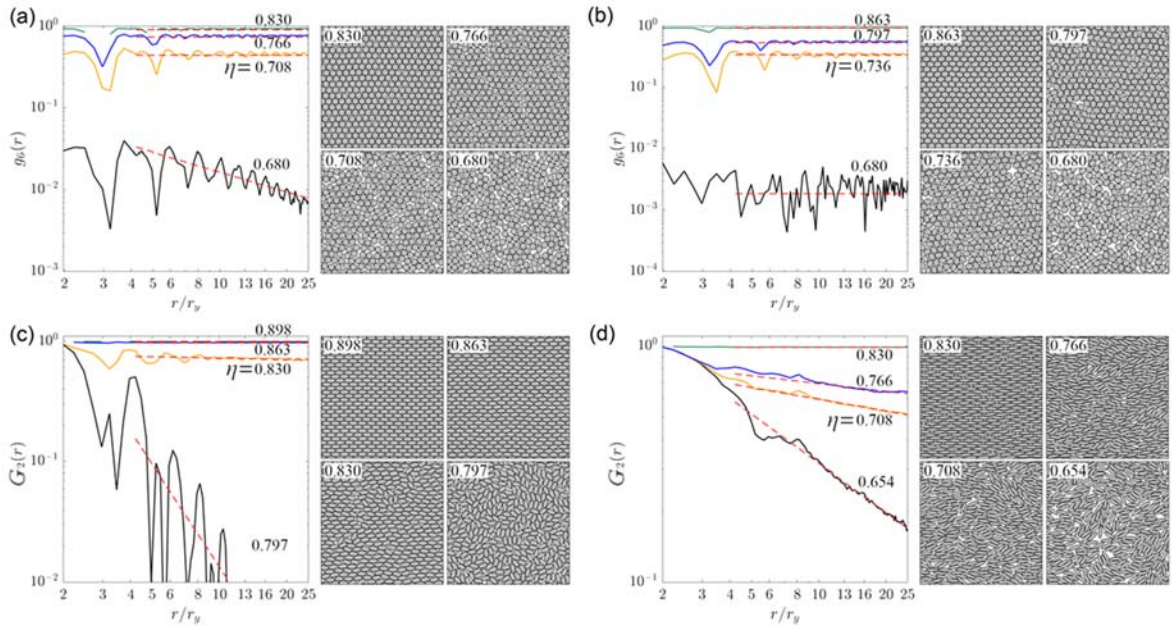


Fig. S3. Orientational correlation functions for several illustrative particle shapes and concentrations. Plots of $g_6(r)$ for (a) hard disks (n=2, r_y/r_x=1) and (b) hard ellipses (n=2, r_y/r_x=0.8) and plots of $G_2(r)$ for hard ellipses with (c) (n=2, r_y/r_x=0.5) and (d) (n=2, r_y/r_x=0.25) for different particle concentrations. Red lines indicate fit slopes at long distances.

Phase		Positional Order	Particle Orientational Order $i = 0,1,2...$	Bond Orientational Order $i = 0,1,2...$	Long range decay of orientational order correlation function	Order Parameters (Constraints)
Liquid	-	None	None	None	$1+\kappa_6 < 0.75$ $1+\kappa_4 < 0.5$ $1+\kappa_2 < 0.75$	-
Liquid Crystal	Nematic	None	$180°\times i$	None	$1+\kappa_2 \geq 0.75$	-
	Tetratic	None	$90°\times i$	None	$1+\kappa_4 \geq 0.5$	$T_4 > 0.5,\ S_2 < 0.5$
	Hexatic	None	-	$60°\times i$	$1+\kappa_6 \geq 0.75$	$\left(r_y/r_x \approx 1,\ n \approx 2\right)$
	Smectic	1-D	$180°\times i$	$180°\times i$	-	$S_2 > 0.5,\ \sigma > 0.5$
Plastic Crystal	-	2-D	None	$60°\times i$	$1+\kappa_6 \geq 0.75$	$S_2 < 0.5,$ $\left(r_y/r_x \neq 1 \text{ or } n \neq 2\right)$
Crystal	4-Fold	2-D	$180°\times i$, or $90°\times i$	$90°\times i$	$1+\kappa_4 \geq 0.99$	$\Psi_4 > \Psi_6$ $\left(\text{if } r_y/r_x \neq 1 \text{ or } n \neq 2: S_2 > 0.5\right)$
	6-Fold	2-D	$180°\times i$, or -	$60°\times i$	$1+\kappa_6 \geq 0.99$	$\Psi_6 > \Psi_4$ $\left(\text{if } r_y/r_x \neq 1 \text{ or } n \neq 2: S_2 > 0.5\right)$

Table S1. For each phase, identification criteria based on union of inequality thresholds for orientation correlation functions and order parameters.

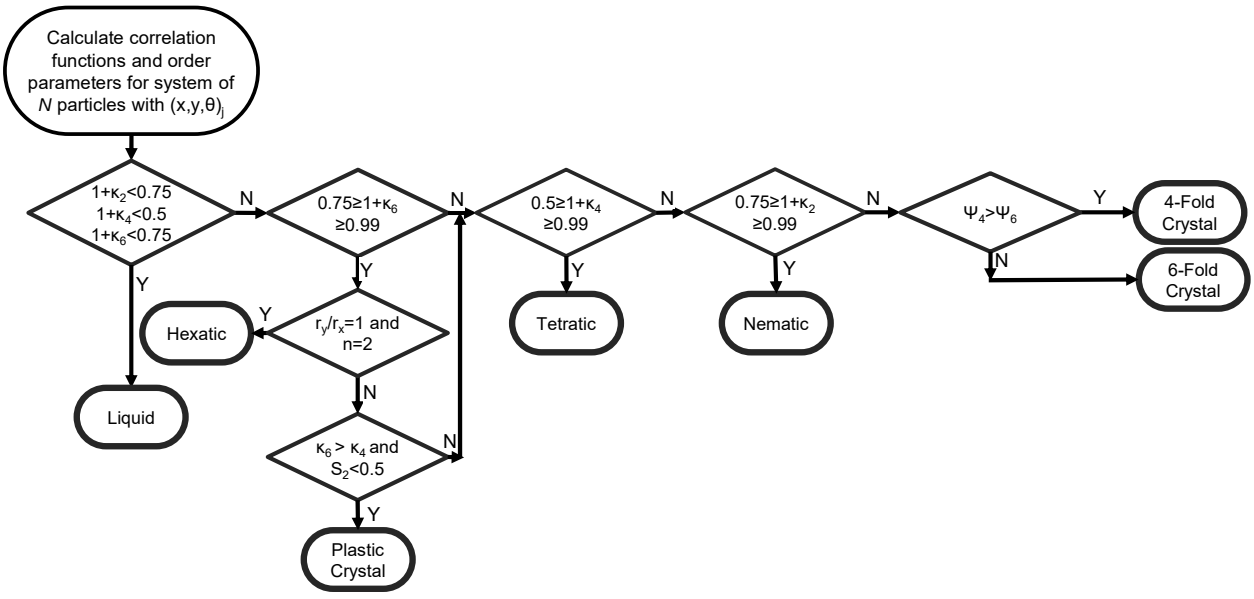


Fig. S4. Flowchart for phase determination based on logic steps using inequality thresholds for orientation correlation functions and order parameters in **Table S1**.

Phase		Positional Order	Particle Orientational Order $i = 0,1,2...$	Bond Orientational Order $i = 0,1,2...$	Order Parameters (Constraints)	
					Position and Orientation	Bond Order
Liquid	-	None	None	None	$\mathrm{All} < 0.5$	$\mathrm{All} < 0.5$
Liquid Crystal	Nematic	None	$180° \times i$	None	$S_2 < 0.5$ $\mathrm{All\ else} < S_2$	$\mathrm{All} < 0.5$
	Tetratic	None	$90° \times i$	None	$T_4 > 0.5,\ S_2 < 0.5$	$\mathrm{All} < 0.5$
	Hexatic	None	-	$60° \times i$	$\left(r_y/r_x \approx 1,\ n \approx 2\right)$	$\Psi_6 > 0.5$
	Smectic	1-D	$180° \times i$	$180° \times i$	$\sigma > 0.5$	$\mathrm{All} < 0.5$
Plastic Crystal	-	2-D	None	$60° \times i$	$\mathrm{All} < 0.5,$ $\left(r_y/r_x \neq 1 \text{ or } n \neq 2\right)$	$\Psi_6 \gtrsim 0.6$
Crystal	4-Fold	2-D	$180° \times i$, or $90° \times i$	$90° \times i$	$\left(\begin{array}{c}\text{if } r_y/r_x \neq 1 \text{ or } n \neq 2: \\ S_2 > 0.5\end{array}\right)$	$\Psi_4 \gtrsim 0.6$ $\left(\begin{array}{c}\text{if } \Psi_6 > 0.2: \\ \Psi_4 > \Psi_6 \text{ and} \\ \Psi_4 + \Psi_6 > 1.2\end{array}\right)$
	6-Fold	2-D	$180° \times i$, or -	$60° \times i$	$\left(\begin{array}{c}\text{if } r_y/r_x \neq 1 \text{ or } n \neq 2: \\ S_2 > 0.5\end{array}\right)$	$\Psi_6 \gtrsim 0.6$ $\left(\begin{array}{c}\text{if } \Psi_4 > 0.2: \\ \Psi_6 > \Psi_4 \text{ and} \\ \Psi_4 + \Psi_6 > 1.2\end{array}\right)$

Table S2. For each phase, approximate identification criteria based on union of inequality thresholds for order parameters based on particle positional, particle orientational, and bond orientational order.

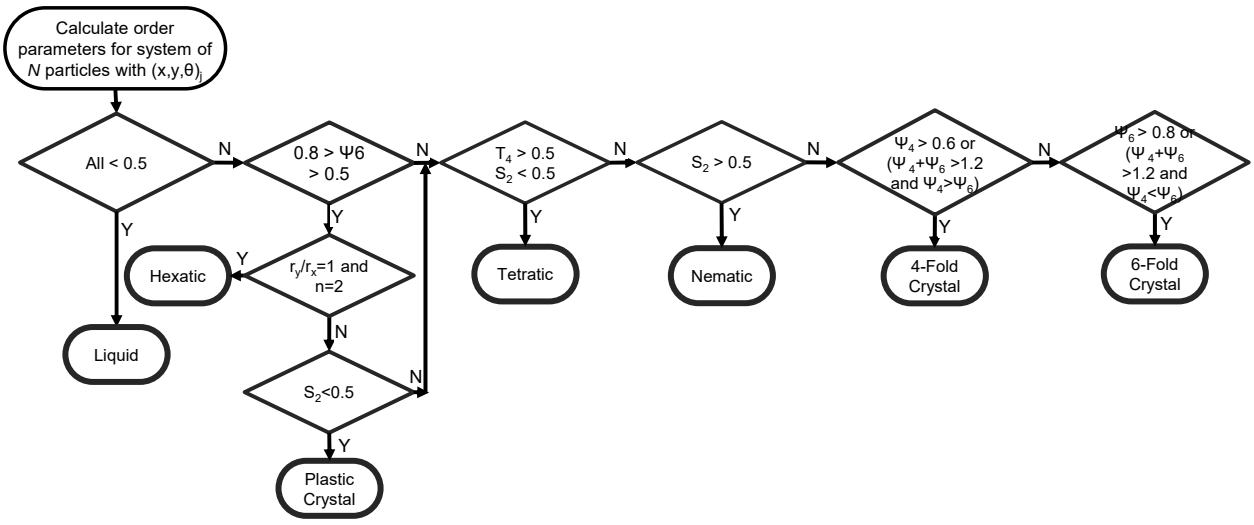


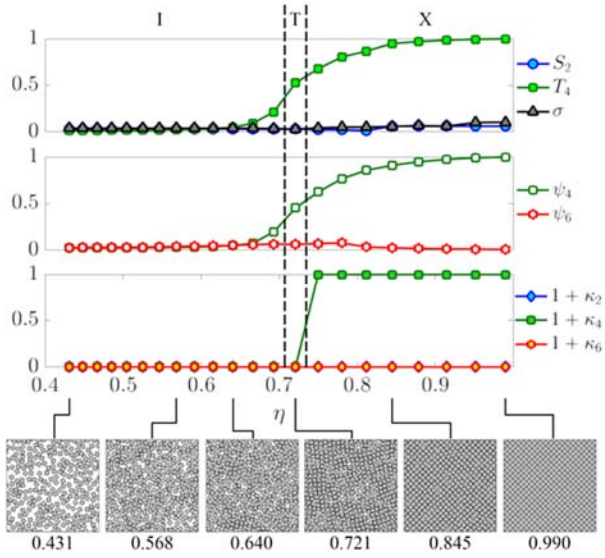
Fig. S5. Flowchart for phase determination based on logic steps using inequality thresholds for order parameters in **Table S2.**

3. Rhombuses (n=1, r_y/r_x=1-0.2)

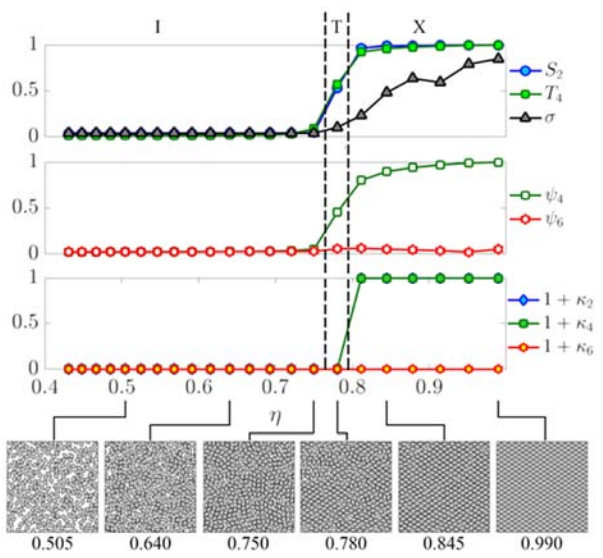
The following caption applies to the remainder of the figures (with exceptions noted).

From top-to-bottom: (a) Nematic, S_2, tetratic, T_4, and smectic, σ, order parameters as a function of particle concentration. (b) Stretched four–fold ψ_4^s and six–fold ψ_6^s symmetry, and (c) long-range power-law decay (κ_2, κ_4, κ_6) for orientational correlation functions. Lower panels are renderings at different particle concentrations at equilibrium conditions. I: Isotropic, N: Nematic, T: Tetratic, P: Plastic crystal, X: Crystal.

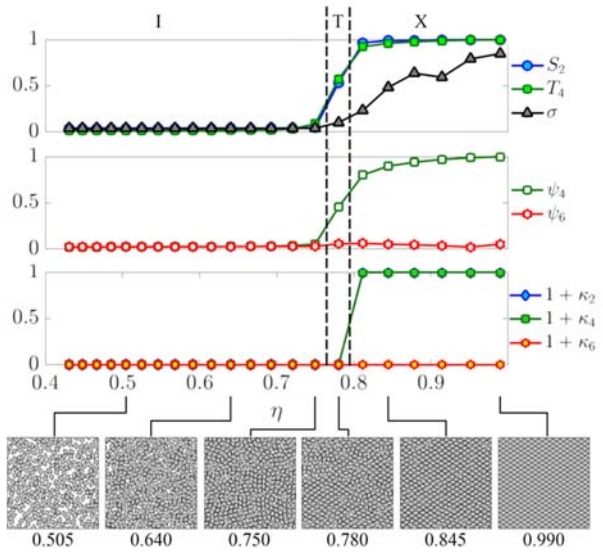
n=1, r_y/r_x=1



n=1, r_y/r_x=0.8



n=1, r_y/r_x=0.67



n=1, r_y/r_x=0.57

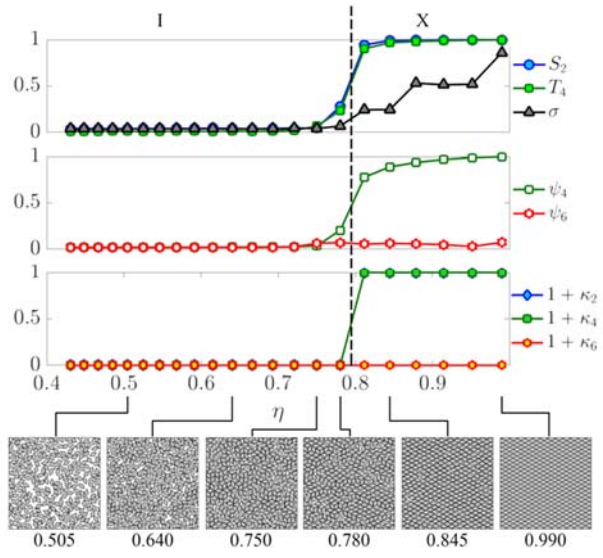
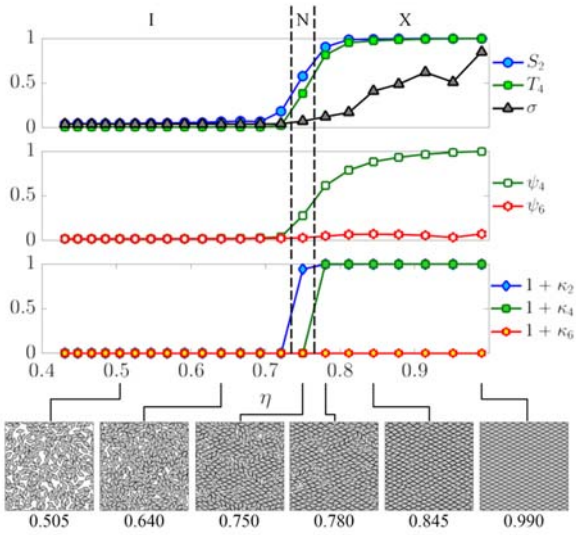
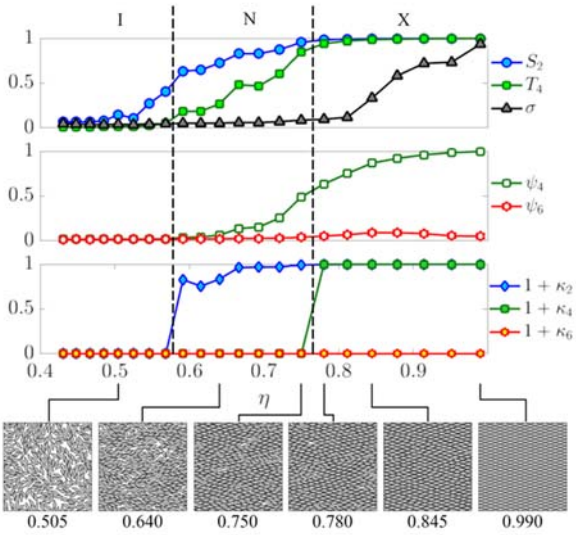


Fig. S6 (a-d). For rhombuses (n=1), order parameters, local symmetry, and correlation function decay (left-to-right, top-to-bottom): (a) r_y/r_x=1, (b) r_y/r_x=0.8, (c), r_y/r_x=0.67, (d) r_y/r_x=0.57.

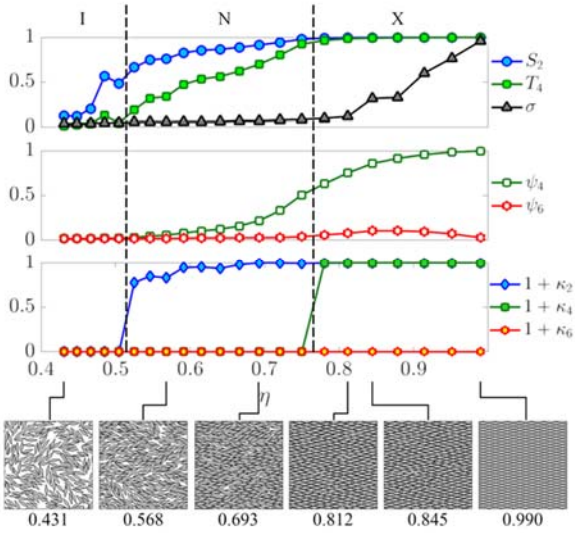
n=1, r_y/r_x=0.5



n=1, r_y/r_x=0.33



n=1, r_y/r_x=0.25



n=1, r_y/r_x=0.2

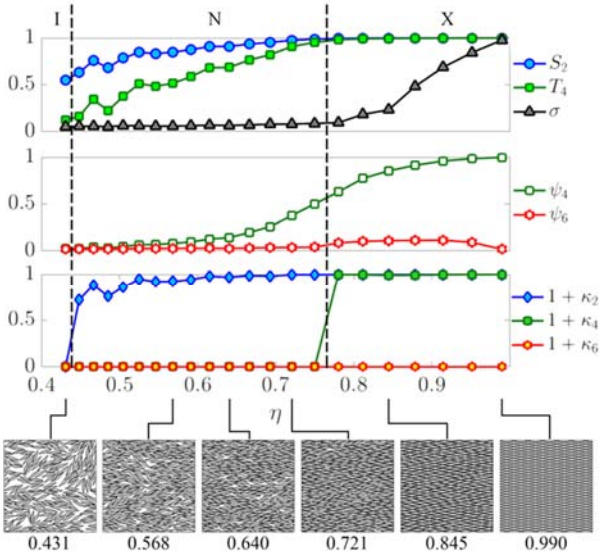


Fig. S6 (e-h). For rhombuses (n=1), order parameters, local symmetry, and correlation function decay (left-to-right, top-to-bottom): (e) r_y/r_x=0.5, (f) r_y/r_x=0.33, (g), r_y/r_x=0.25, (h) r_y/r_x=0.2.

4. Rounded Rhombuses (n=1.4, r_y/r_x=1-0.2)

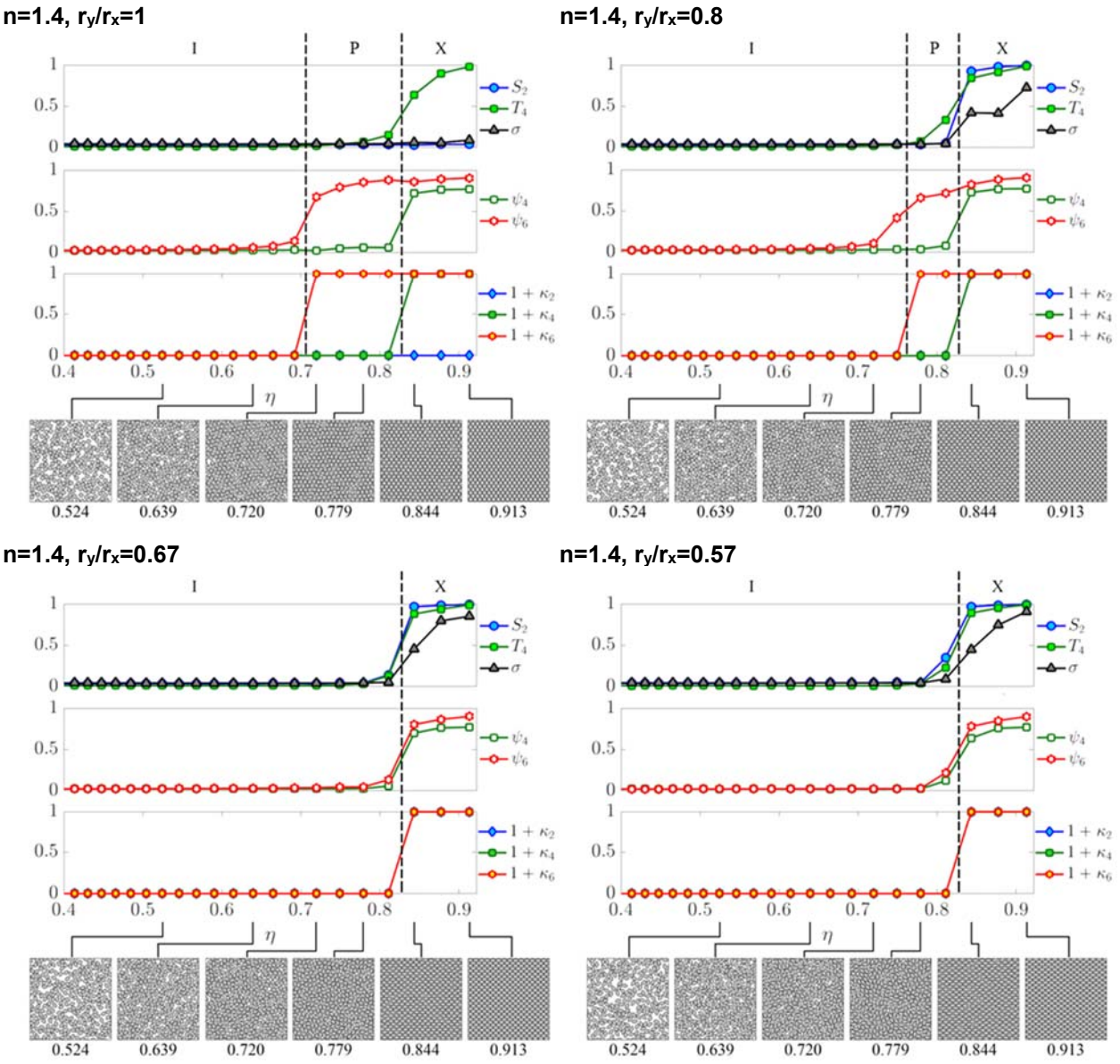


Fig. S7 (a-d). For rounded rhombuses (n=1.4), order parameters, local symmetry, and correlation function decay (left-to-right, top-to-bottom): (a) r_y/r_x=1, (b) r_y/r_x=0.8, (c), r_y/r_x=0.67, (d) r_y/r_x=0.57.

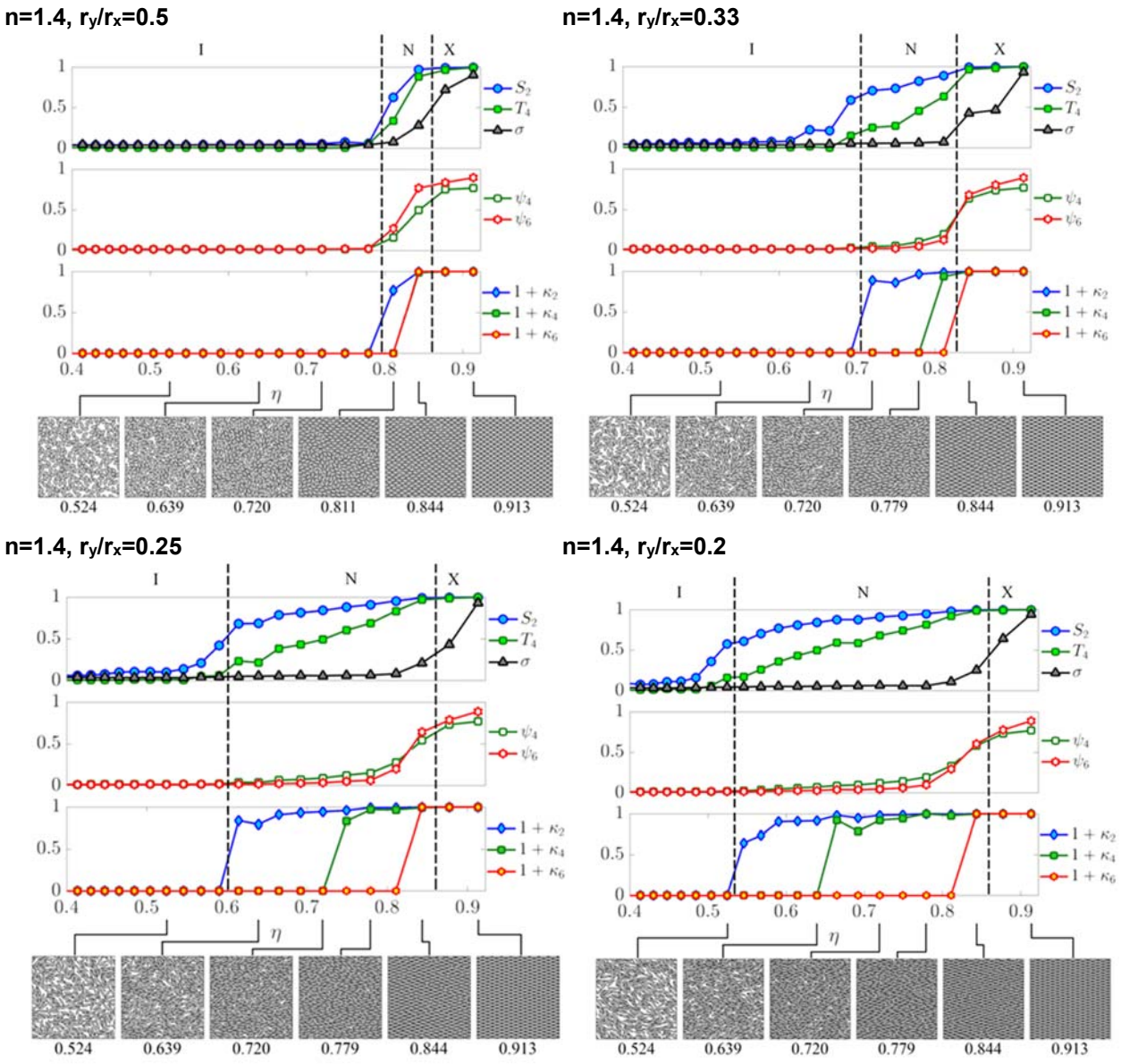


Fig. S7 (e-h). For rounded rhombuses (n=1.4), order parameters, local symmetry, and correlation function decay (left-to-right, top-to-bottom): (e) r_y/r_x=0.5, (f) r_y/r_x=0.33, (g), r_y/r_x=0.25, (h) r_y/r_x=0.2.

5. Ellipses (n=2, r_y/r_x=1-0.2)

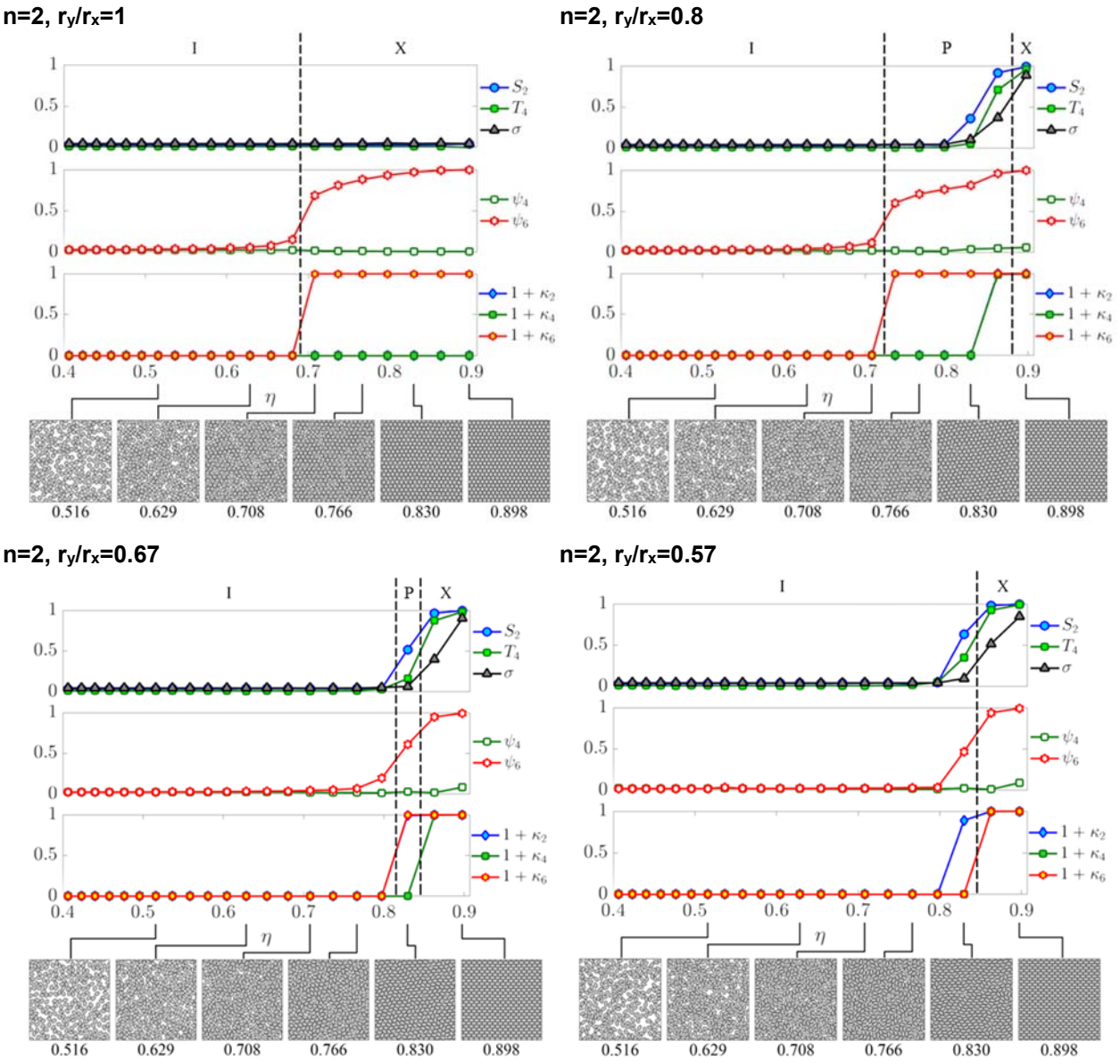


Fig. S8 (a-d). For ellipses (n=2), order parameters, local symmetry, and correlation function decay (left-to-right, top-to-bottom): (a) r_y/r_x=1, (b) r_y/r_x=0.8, (c), r_y/r_x=0.67, (d) r_y/r_x=0.57.

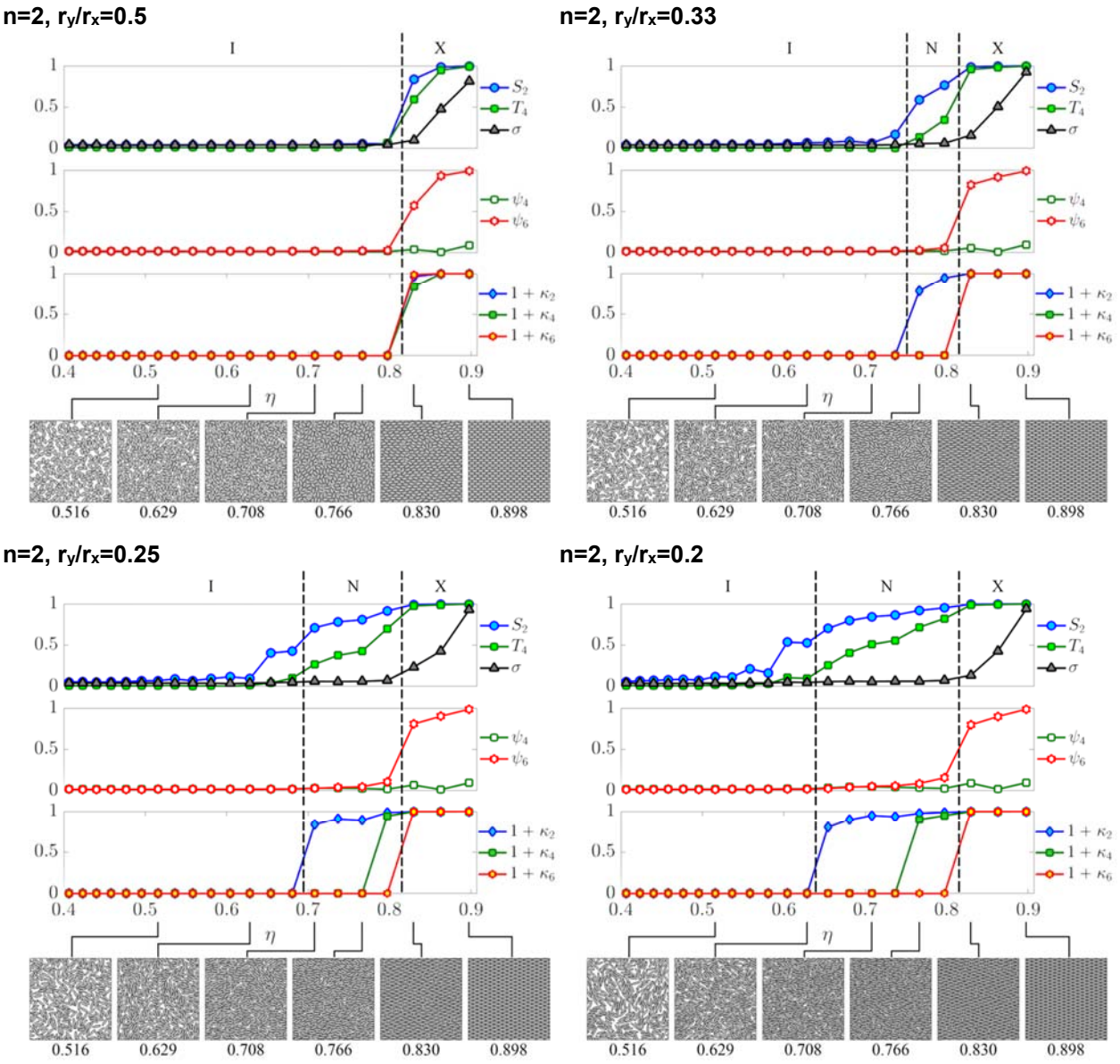


Fig. S8 (e-h). For ellipses (n=2), order parameters, local symmetry, and correlation function decay (left-to-right, top-to-bottom): (e) r_y/r_x=0.5, (f) r_y/r_x=0.33, (g), r_y/r_x=0.25, (h) r_y/r_x=0.2.

6. Rounded Rectangles (n=4, r_y/r_x=1-0.2)

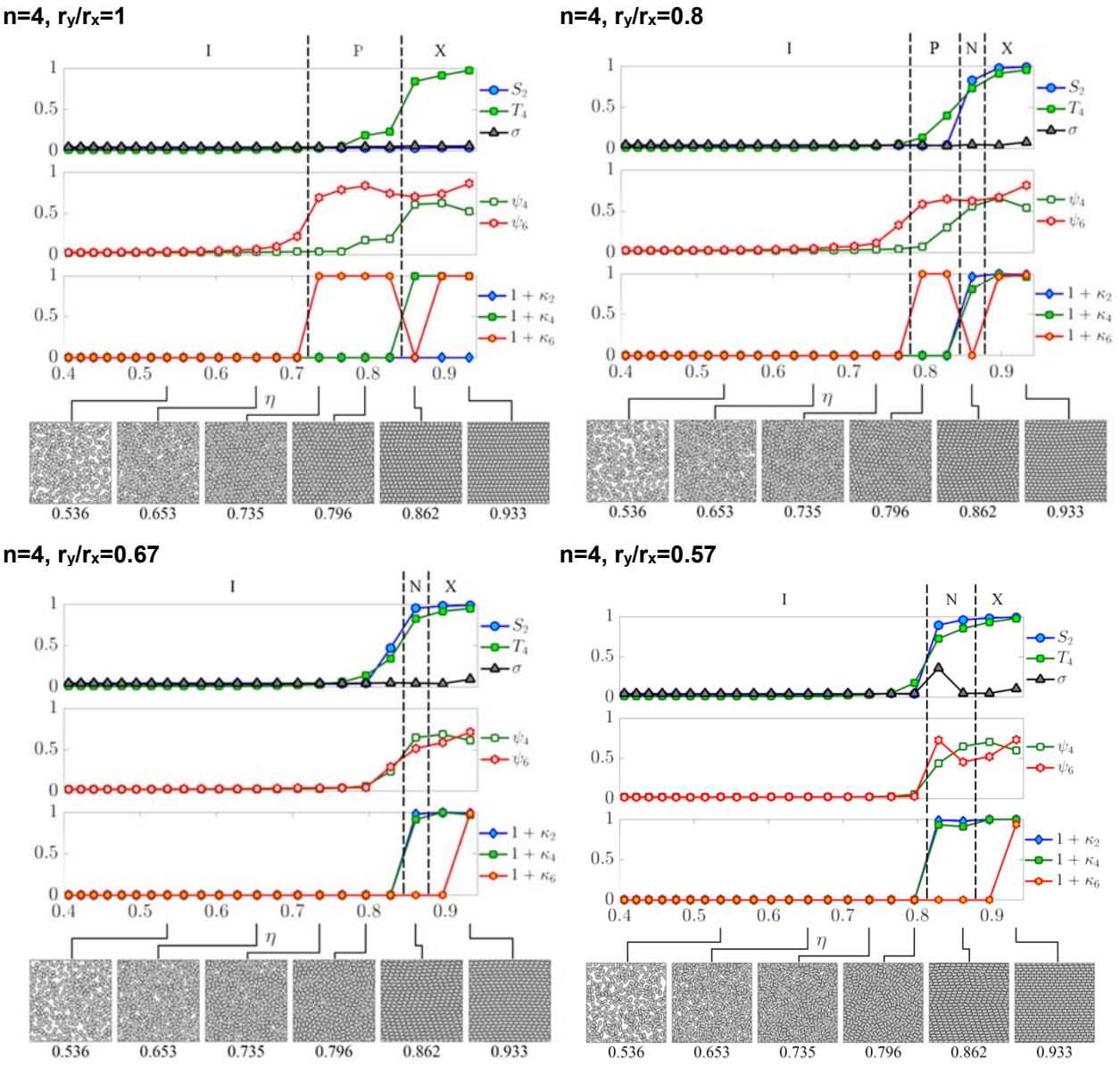


Fig. S9 (a-d). For rounded rectangles (n=4), order parameters, local symmetry, and correlation function decay (left-to-right, top-to-bottom): (a) r_y/r_x=1, (b) r_y/r_x=0.8, (c), r_y/r_x=0.67, (d) r_y/r_x=0.57.

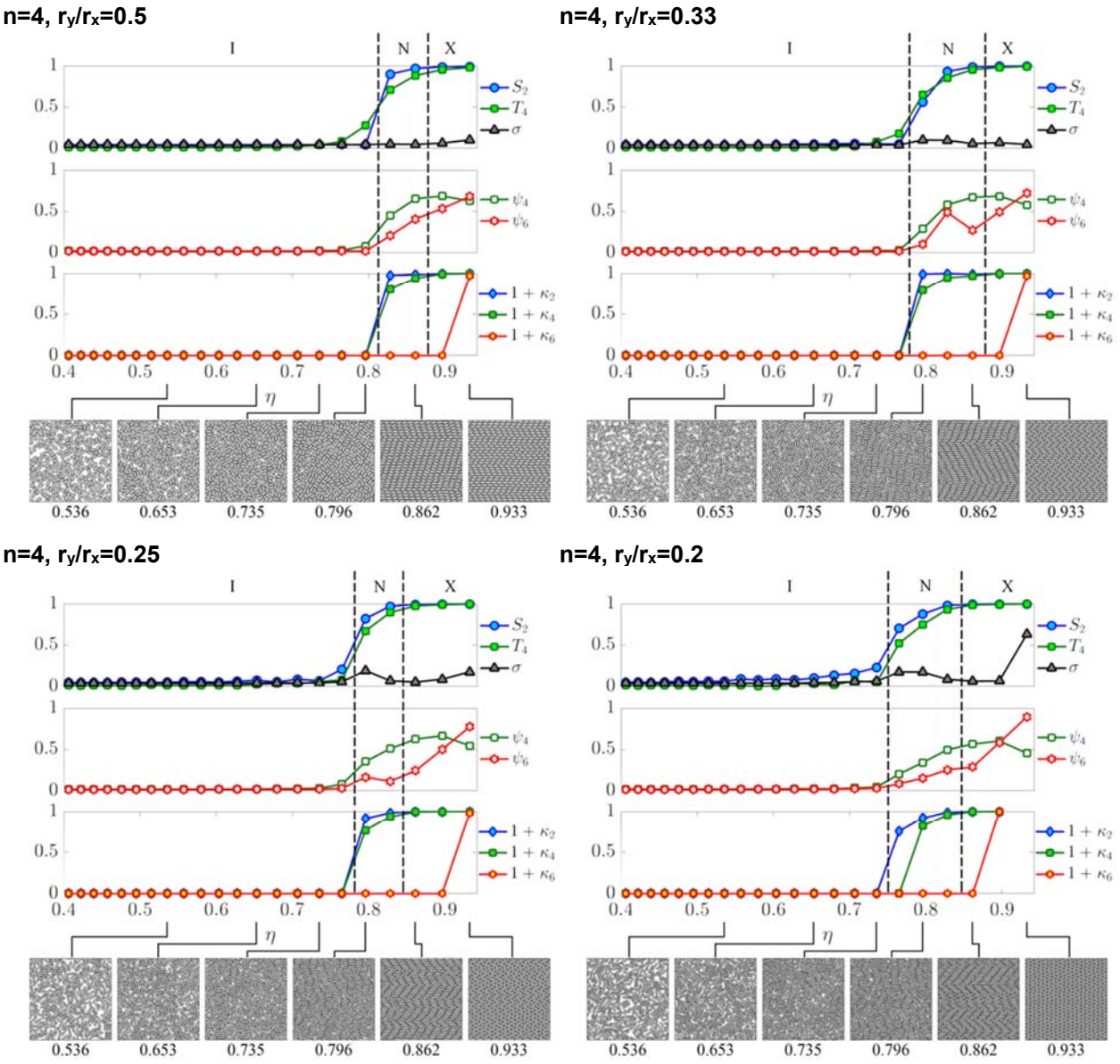


Fig. S9 (e-h). For rounded rectangles (n=4), order parameters, local symmetry, and correlation function decay (left-to-right, top-to-bottom): (e) r_y/r_x=0.5, (f) r_y/r_x=0.33, (g), r_y/r_x=0.25, (h) r_y/r_x=0.2.

7. Rectangles (n=∞, r_y/r_x=1-0.2)

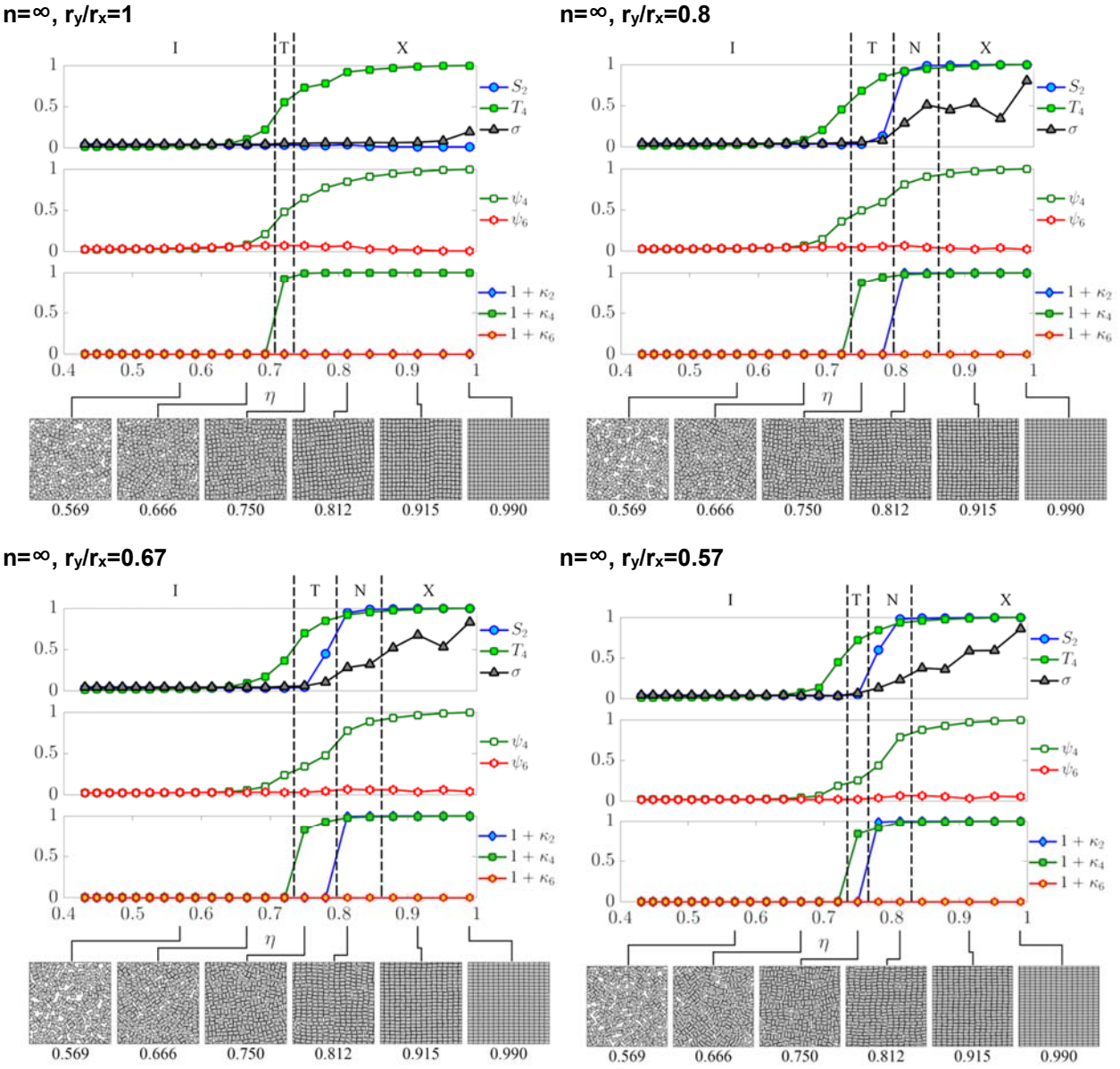


Fig. S10 (a-d). For rectangles (n=∞), order parameters, local symmetry, and correlation function decay (left-to-right, top-to-bottom): (a) r_y/r_x=1, (b) r_y/r_x=0.8, (c), r_y/r_x=0.67, (d) r_y/r_x=0.57.

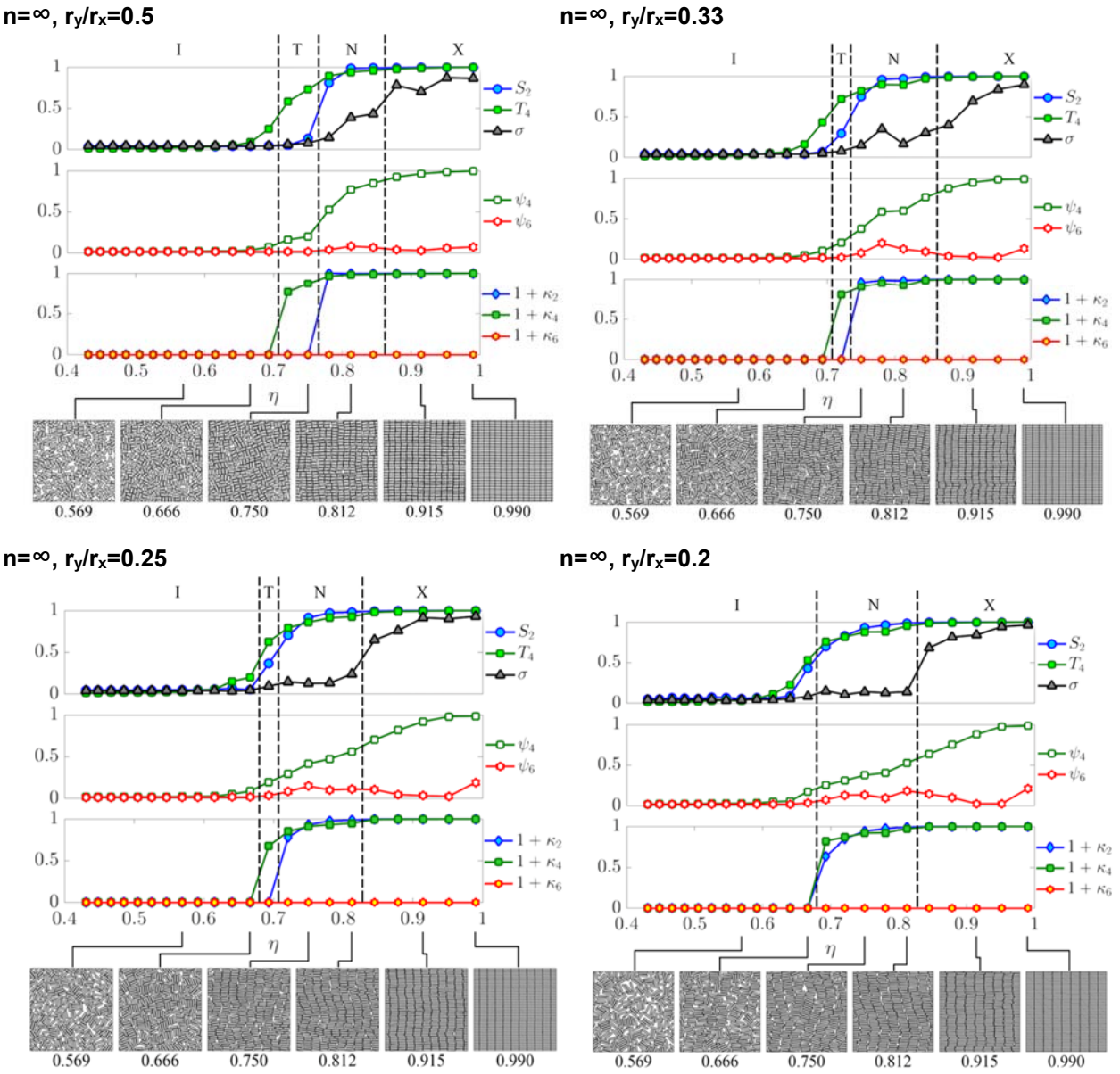


Fig. S10 (e-h). For rectangles with (n=∞), order parameters, local symmetry, and correlation function decay (left-to-right, top-to-bottom): (e) r_y/r_x=0.5, (f) r_y/r_x=0.33, (g), r_y/r_x=0.25, (h) r_y/r_x=0.2.