Electronic Supplementary Material (ESI) for Nanoscale.

Electronic Supplementary Information

Kinetics-controlled design principles for two-dimensional open lattices using atom-mimicking patchy particles

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Table S1: The corresponding relation between simulation parameters α_{ij}^R and α_{ij}^A and the experimentally measurable properties E, G, and d_{eff}. The parameters α_{ij}^R, α_{ij}^A, and δ are given in reduced units, and the reduced unit of length d_{ij} in the model is assumed to approximately correspond to 10 nm.

α_{ij}^R	α_{ij}^A	δ	E [Pa]	G [k_BT]	d_{eff} [nm]
396	223	0.220	5.64×10^6	10.00	8.20
490	242	0.198	6.62×10^6	10.00	8.34
621	270	0.179	7.98×10^6	10.00	8.48
1596	400	0.111	1.72×10^7	10.00	9.00

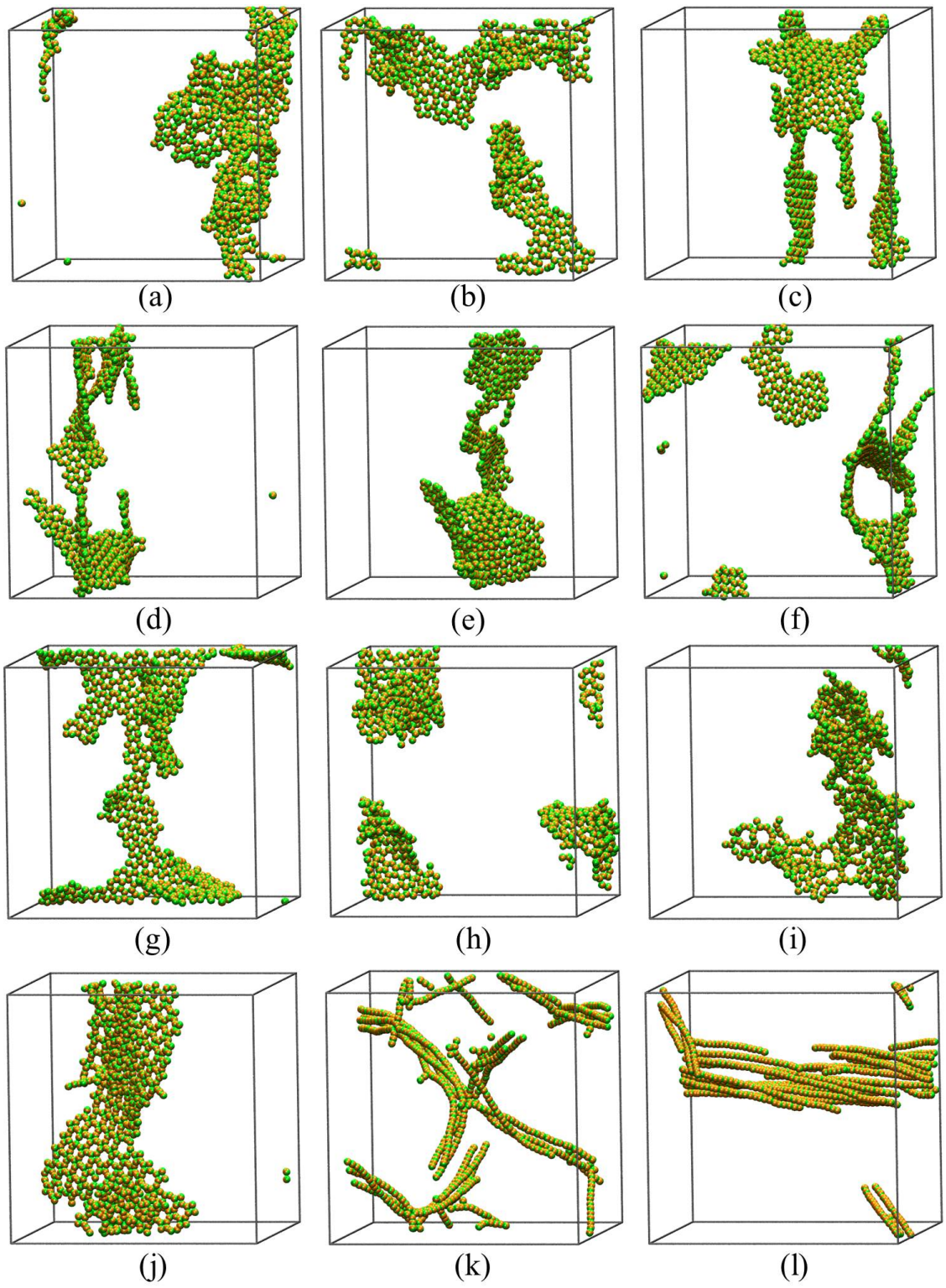

Figure S1: Typical self-assembled structures from soft three-patch particles at different values of φ: (a) $\varphi = 100°$, (b) $\varphi = 105°$, (c) $\varphi = 110°$, (d) $\varphi = 115°$, (e) $\varphi = 120°$, (f) $\varphi = 125°$, (g) $\varphi = 130°$, (h) $\varphi = 135°$, (i) $\varphi = 140°$, (j) $\varphi = 145°$, (k) $\varphi = 150°$, (l) $\varphi = 160°$. For the sake of clarity, we only show patchy solute particles in these systems.

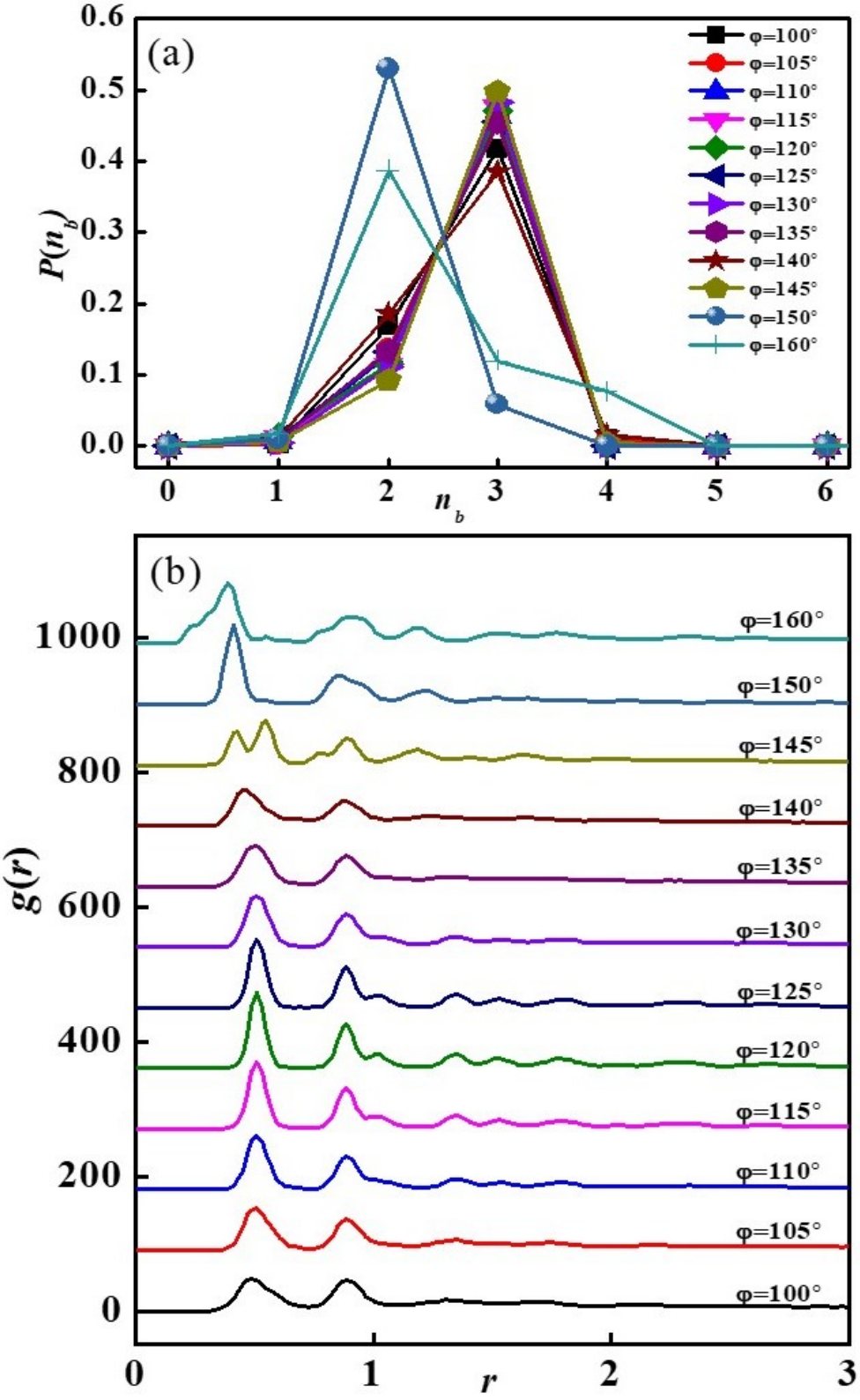

Figure S2: Structural characteristics of typical self-assembled structures in Fig.S1. (a) Probability distribution $P(n_b)$ of the number of bonds (i.e., contacts) n_b between attractive patches per patchy particle. (b) The radial distribution function $g(r)$ (shifted upward for clarity).

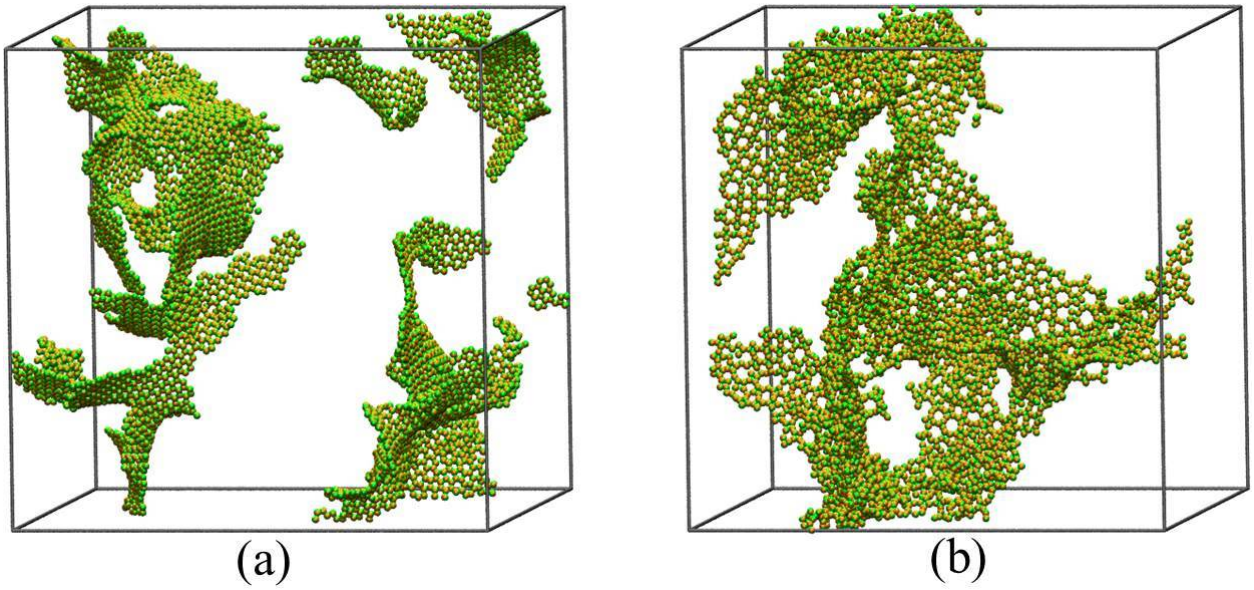

Figure S3: Typical self-assembled structures observed in Fig.2 with larger system size of 1.92×10^5 particles in a $40 \times 40 \times 40$ cubic box. (a) Hexagonal honeycomb lattice. (b) Square-octagon lattice.

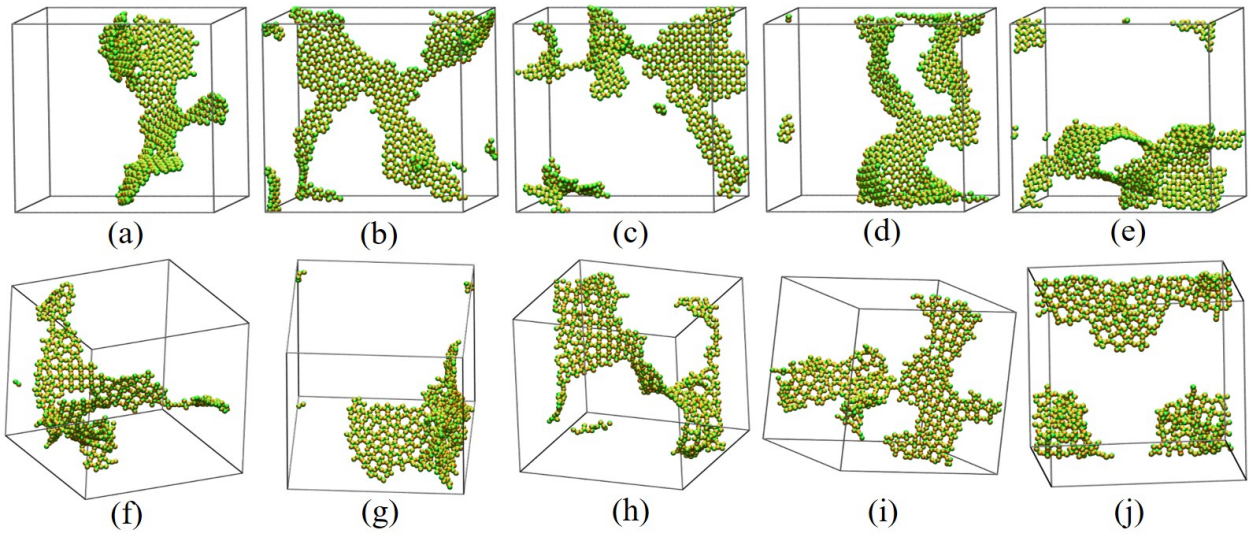

Figure S4: (a)-(e) Hexagonal honeycomb lattice structures for five independent simulations from different initial configurations. (f)-(j) Square-octagon lattice structures for five independent simulations from different initial configurations.

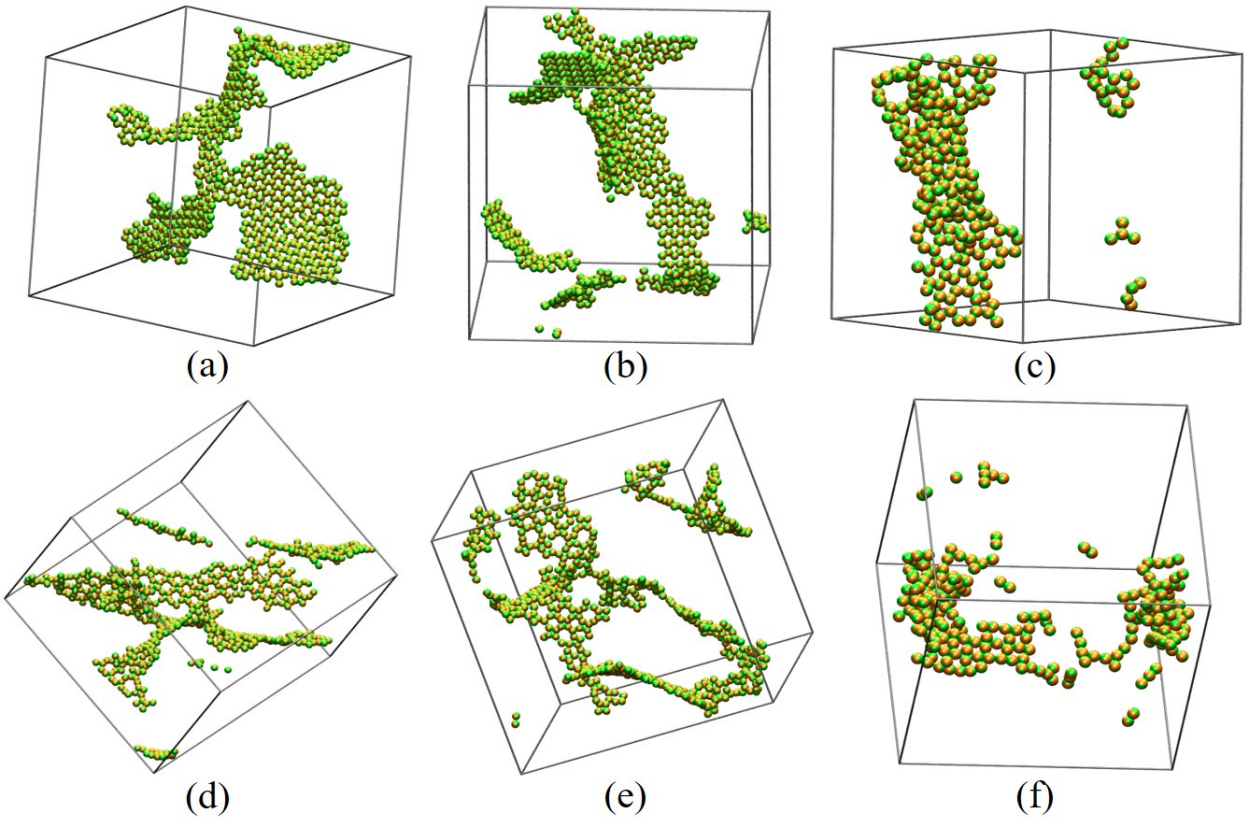

Figure S5: (a)-(c) Typical self-assembled structures for different α_{ij}^{R} with keeping $G \approx 10.00\ k_BT$, $\theta_m^{\kappa} = 45^{\circ}$ and $\varphi = 120^{\circ}$: (a) honeycomb lattice at $\alpha_{ij}^{R} = 490$ ($E \approx 6.6$ Mpa), (b) honeycomb lattice at $\alpha_{ij}^{R} = 621$ ($E \approx 8.0$ Mpa), (c) disordered network structures at $\alpha_{ij}^{R} = 1596$ ($E \approx 17.2$ Mpa). (d)-(f) Typical self-assembled structures for different α_{ij}^{R} with keeping $G \approx 10.00\ k_BT$, $\theta_m^{\kappa} = 45^{\circ}$ and $\varphi = 145^{\circ}$: (d) square-octagon lattice at $\alpha_{ij}^{R} = 490$ ($E \approx 6.6$ Mpa), (e) square-octagon lattice at $\alpha_{ij}^{R} = 621$ ($E \approx 8.0$ Mpa), (f) disordered network structures at $\alpha_{ij}^{R} = 1596$ ($E \approx 17.2$ Mpa).

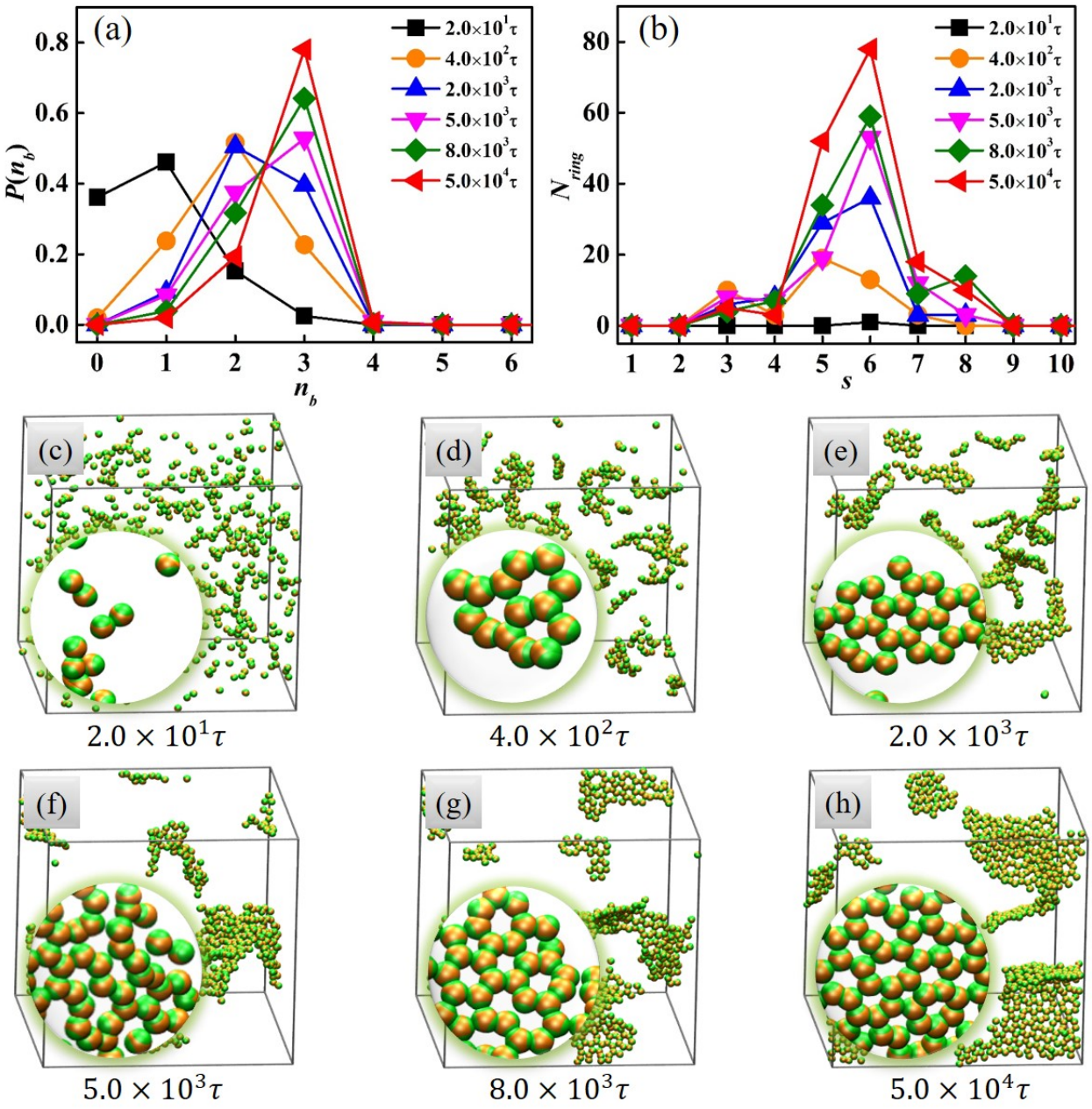

Figure S6: Kinetics of self-assembly of 2D network structures with irregular polygonal pores in Fig.S1h. (a) Probability distribution $P(n_b)$ of the number of bonds n_b between attractive patches per patchy particle at different times. (b) Time evolution of the number N_{ring} of polygonal rings with different size s. (c)-(h)Typical snapshots taken at different times. System of soft three-patch particles with $\alpha_{ij}^R = 396$, $\Phi = 3.0\%$, $G \approx 10.00\ k_BT$, $\theta_m^\kappa = 45^\circ$, and $\varphi = 135^\circ$ is chosen to show the formation kinetics.