

**Supplementary Information**  
**Growth Pathway of AB<sub>2</sub>-Type Colloidal Alloy during Colloidal**  
**Heteroepitaxy**

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TABLE S1. Energy gains caused by the formation of AB<sub>2</sub> structure for the parameter sets used in our simulations, where  $R_{\text{Sub}} = 0.5$ .

$(R_A/R_{\text{Sub}}, R_B/R_{\text{Sub}})$	$\epsilon_{\text{SA}}/\epsilon_0$	$\epsilon_{\text{SB}}/\epsilon_0$	$\epsilon_{\text{AB}}/\epsilon_0$	$\epsilon_A/\epsilon_0$	$\epsilon_B/\epsilon_0$	$\bar{\epsilon}_{\text{AB}_2}/\epsilon_0$
(1.2, 0.8)	0.272	0.222	0.240	1.54	1.03	1.20
(1.15, 0.85)	0.262	0.229	0.244	1.54	1.06	1.22
(1.1, 0.9)	0.261	0.239	0.248	1.53	1.08	1.23
(1.05, 0.95)	0.256	0.243	0.249	1.52	1.10	1.24

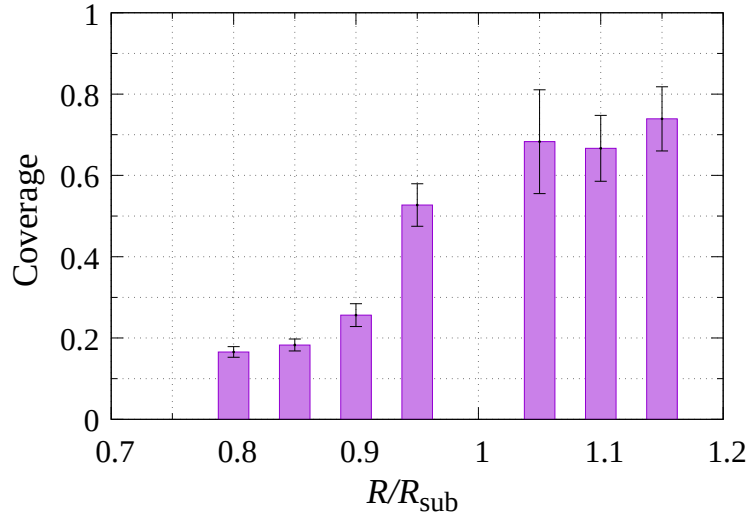


FIG. S1. Dependence of the coverage of the substrate by epitaxial particles on the particle radius  $R$ . The data were averaged over 20 individual runs, which were measured at  $t = 2000$ .

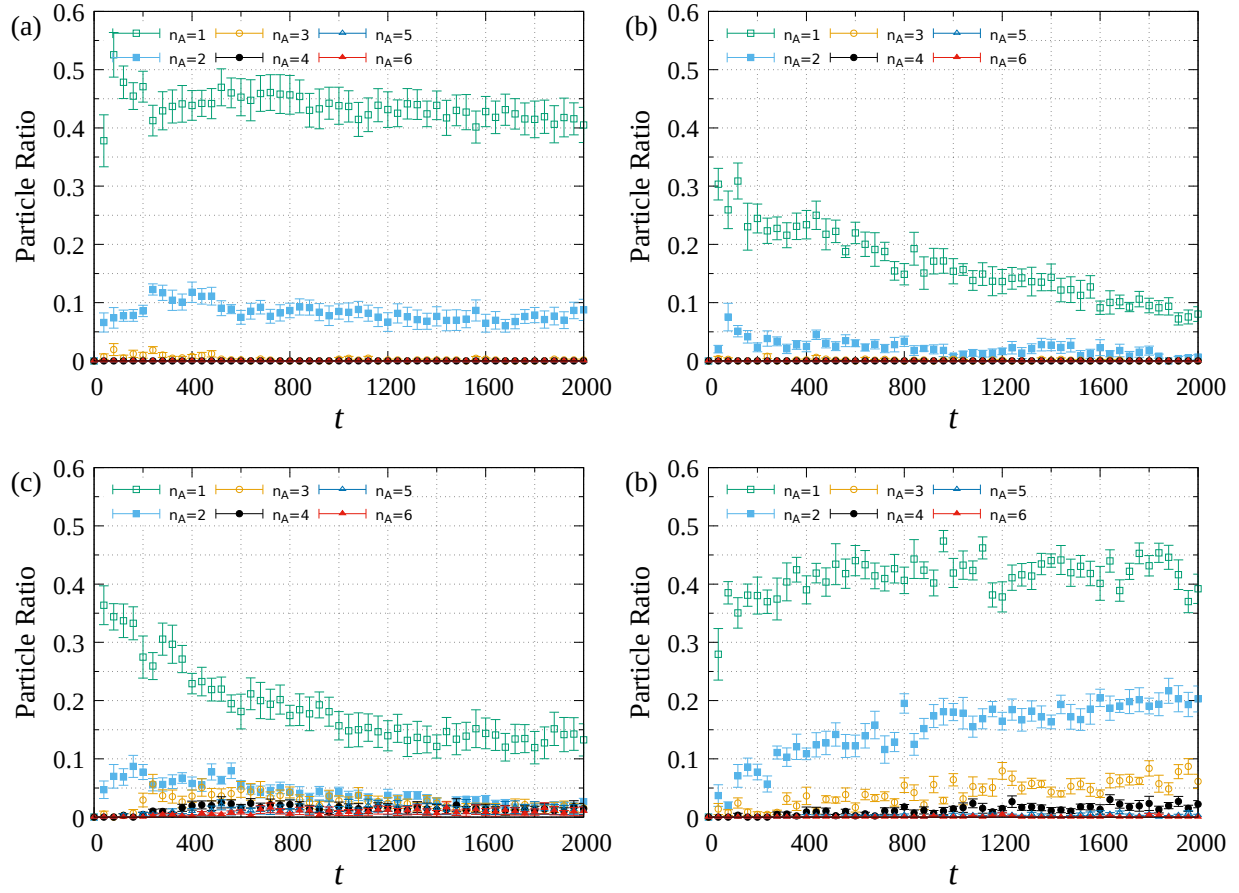


FIG. S2. Time dependence of the fraction of A particles attached to  $n_A$  A particles, normalized by the total number of A particles on the substrate, for different radius ratios  $((R_A/R_{\text{Sub}}, R_B/R_{\text{Sub}})$ : (a) (1.05, 0.95), (b) (1.1, 0.9), (c) (1.15, 0.85), and (d) (1.2, 0.8). The data are averaged over 20 independent runs.

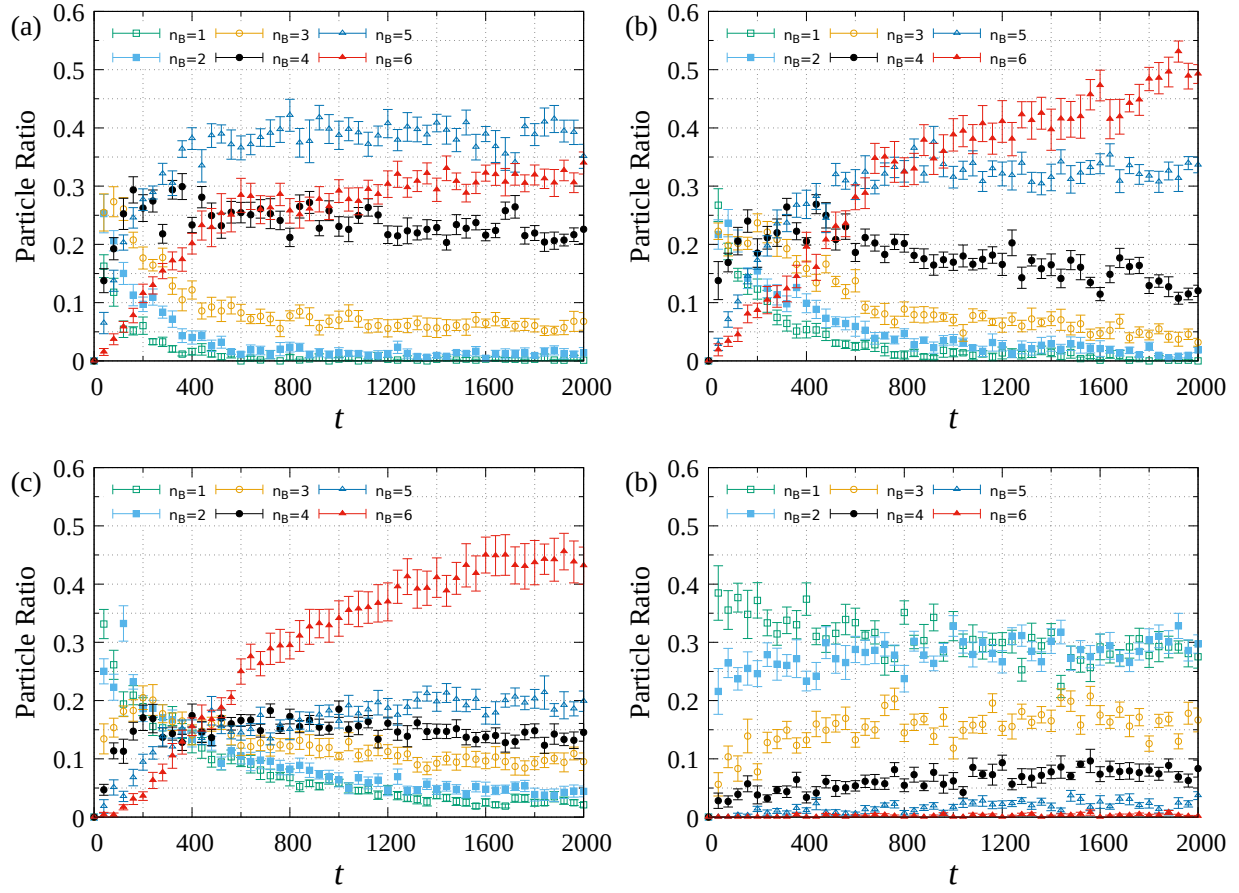


FIG. S3. Time dependence of the fraction of A particles attached to  $n_B$  B particles, normalized by the total number of A particles on the substrate, for different radius ratios  $((R_A/R_{\text{Sub}}, R_B/R_{\text{Sub}})$ : (a) (1.05, 0.95), (b) (1.1, 0.9), (c) (1.15, 0.85), and (d) (1.2, 0.8). The data are averaged over 20 independent runs.

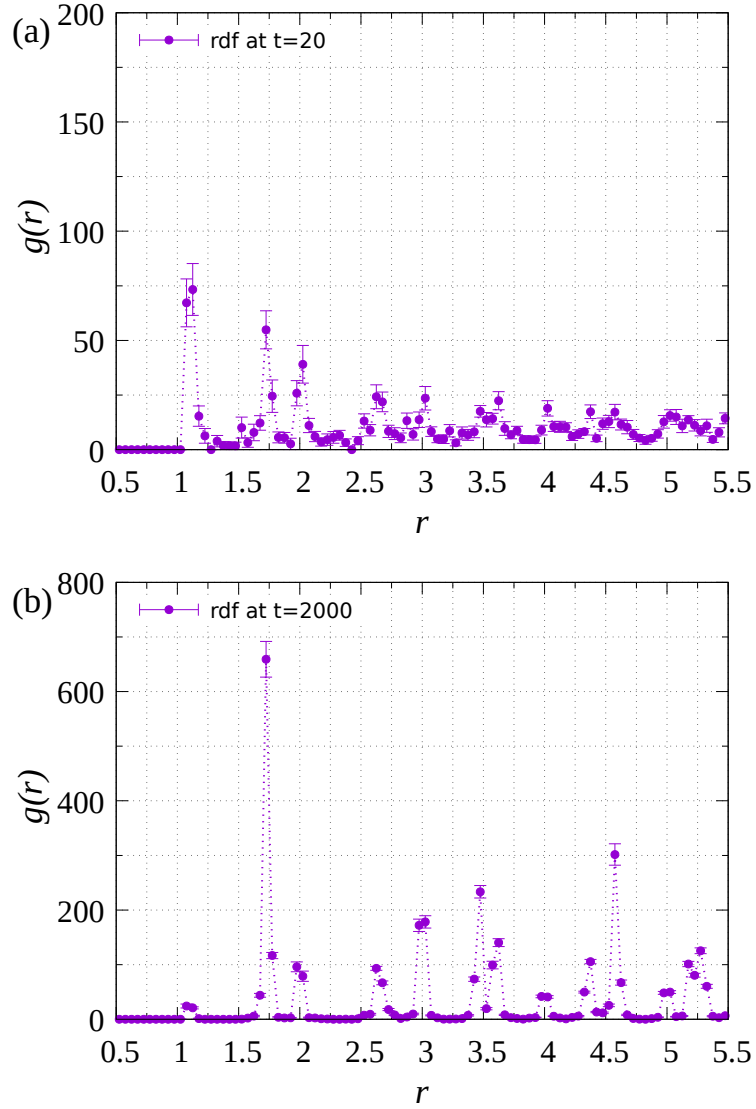


FIG. S4. Radial distribution functions  $g(r)$  for  $(R_A/R_{\text{Sub}}, R_B/R_{\text{Sub}}) = (1.1, 0.9)$  with  $N_A = 200$  and  $N_B = 600$  at (a)  $t = 20$  and (b)  $t = 2000$ .

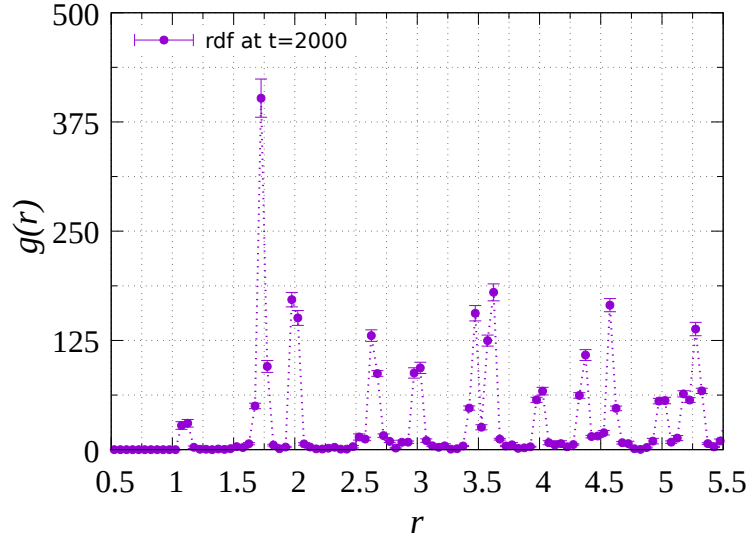


FIG. S5. Radial distribution function for  $(R_A/R_{\text{Sub}}, R_B/R_{\text{Sub}}) = (1.1, 0.9)$  with  $N_A = 200$  and  $N_B = 1200$  at  $t = 2000$ .