Electronic Supplementary Information

A simulation model for soft triblock Janus particles and their ordered packing

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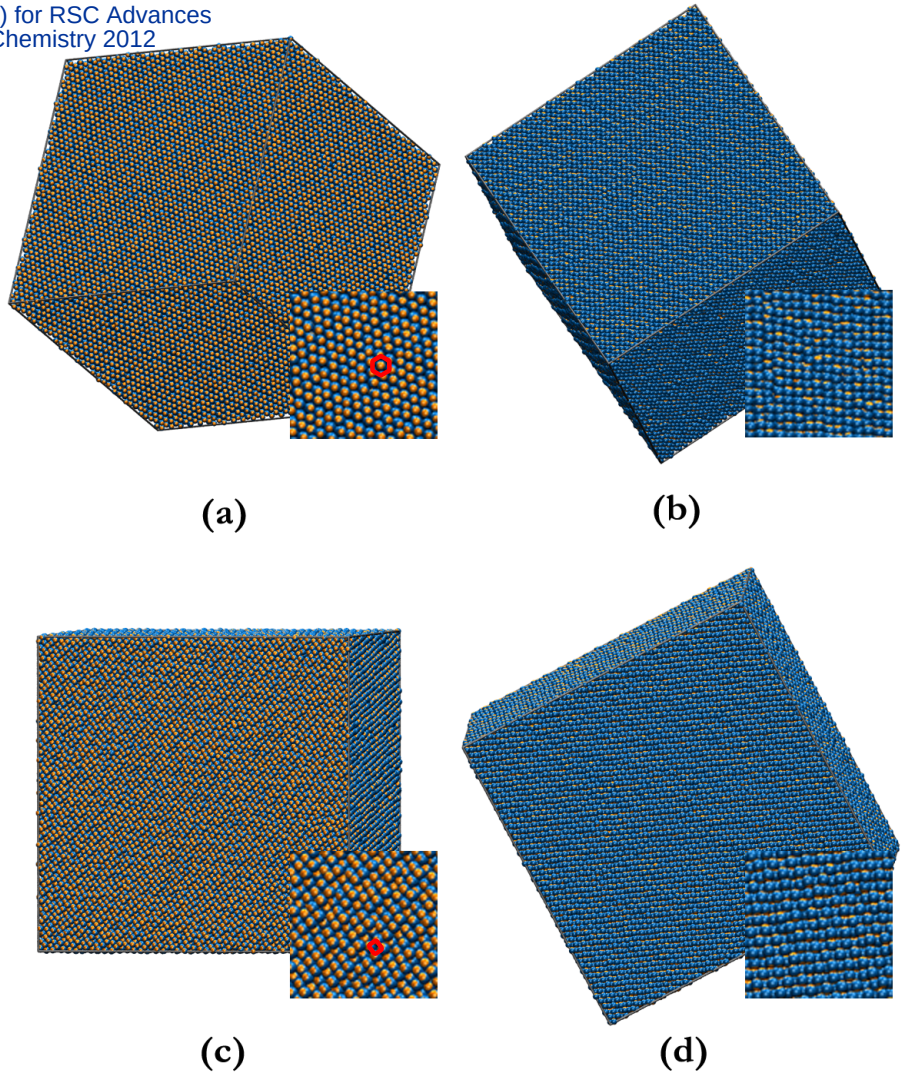

Figure S1: Typical packing structures for larger system size with 1.92×10^5 particles in a $40 \times 40 \times 40$ cubic box. In these systems, $\alpha_{ij}^R = 396$, $\alpha_{ij}^A = 88$, and $\nu = 0.5$, but β is different. (a) Top view of hexagonal columnar structure ($\beta = 45^\circ$), (b) side view of (a), (c) top view of body-centered tetragonal structure ($\beta = 60^\circ$), (d) side view of (c).

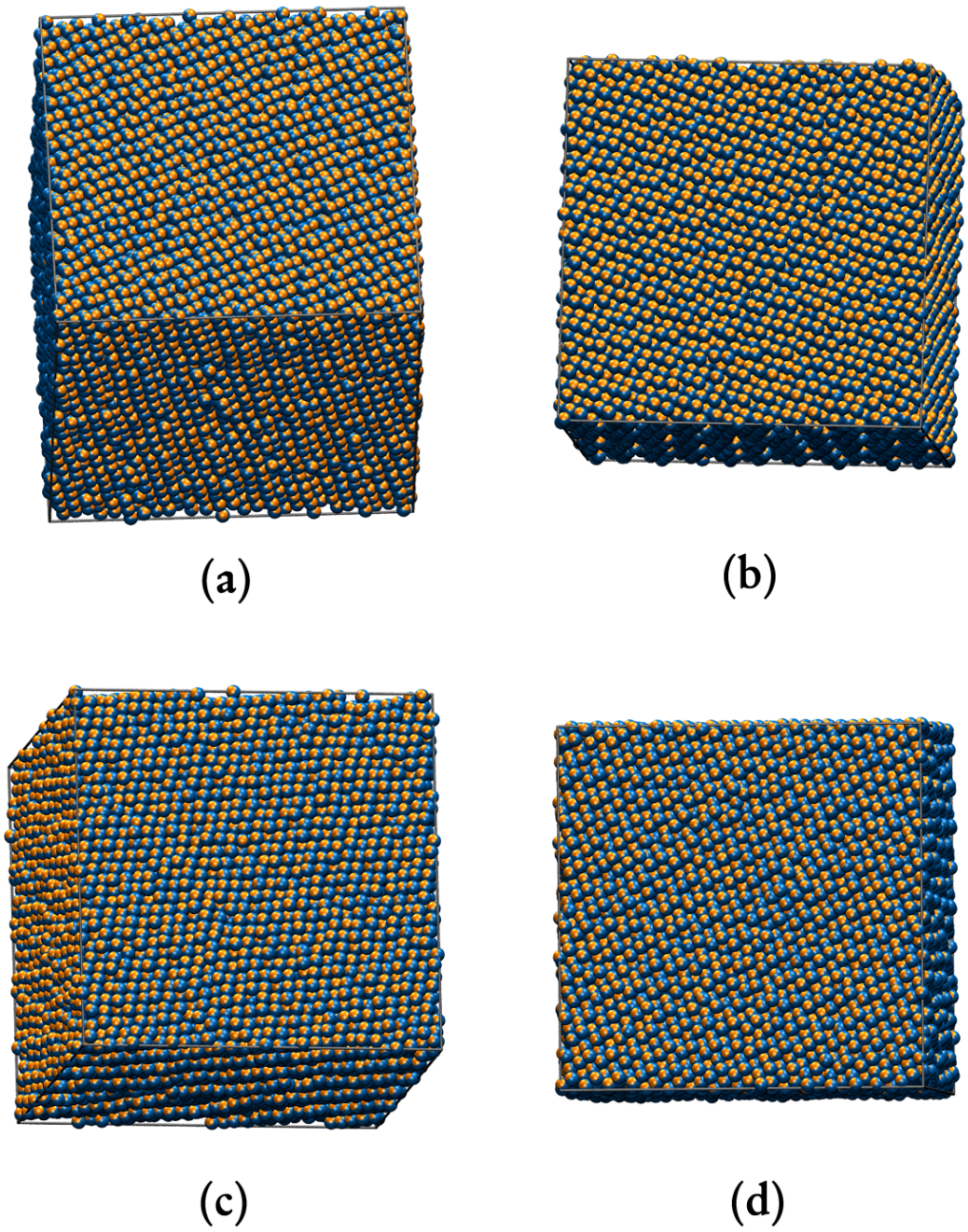

Figure S2: The ordered BCT packing structures for four independent simulations from different initial configurations. In these systems, $\alpha_{ij}^{R} = 396$, $\alpha_{ij}^{A} = 88$, $\nu = 0.5$, and $\beta = 60^{\circ}$.

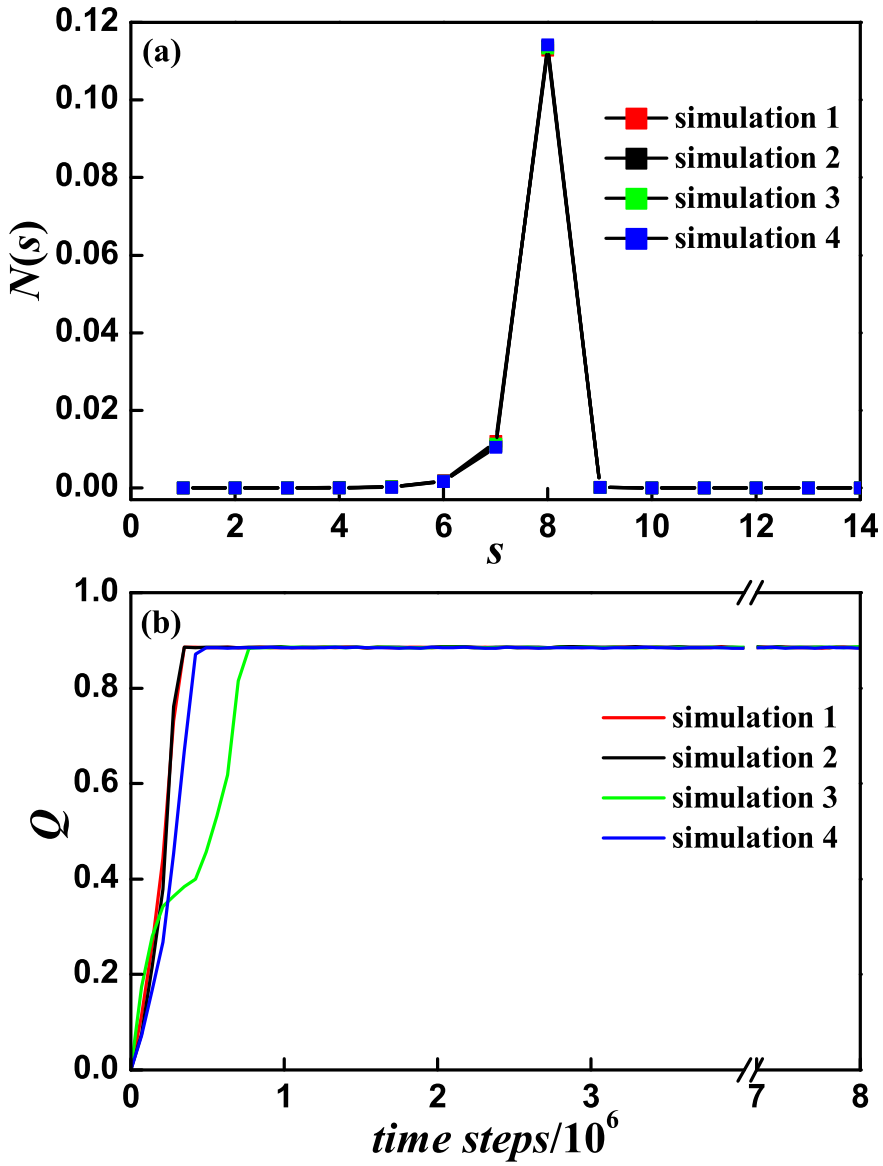

Figure S3: (a) Distribution $N(s)$ of the number of contacts s, and (b) the time evolution of the orientation order parameter Q for four independent simulations from different initial configurations while keeping $\alpha_{ij}^{R} = 396$, $\alpha_{ij}^{A} = 88$, $\nu = 0.5$, and $\beta = 60°$. It should be noted that the distribution $N(s)$ and the orientation order parameter Q after equilibrium for four independent simulations are almost overlapped.

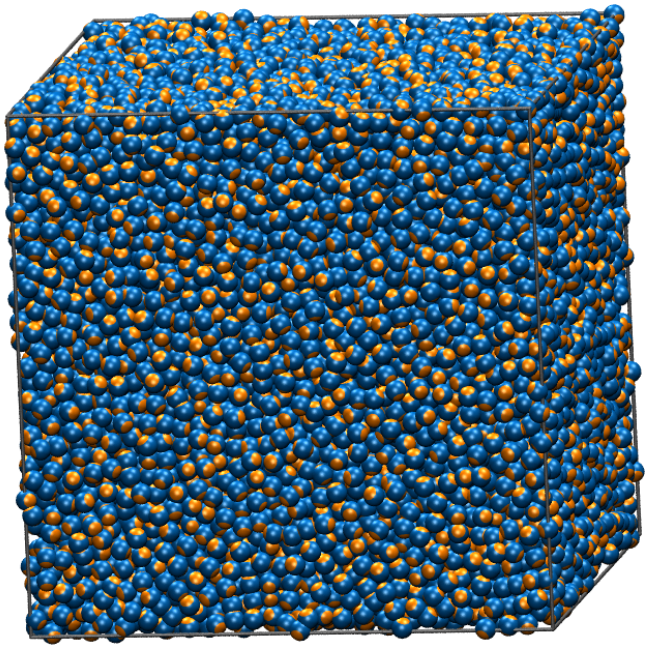

Figure S4: The packing structure for very small α_{ij}^{A}. In this system, $\alpha_{ij}^{R} = 396$, $\alpha_{ij}^{A} = 44$, $\nu = 0.5$, and $\beta = 45°$.

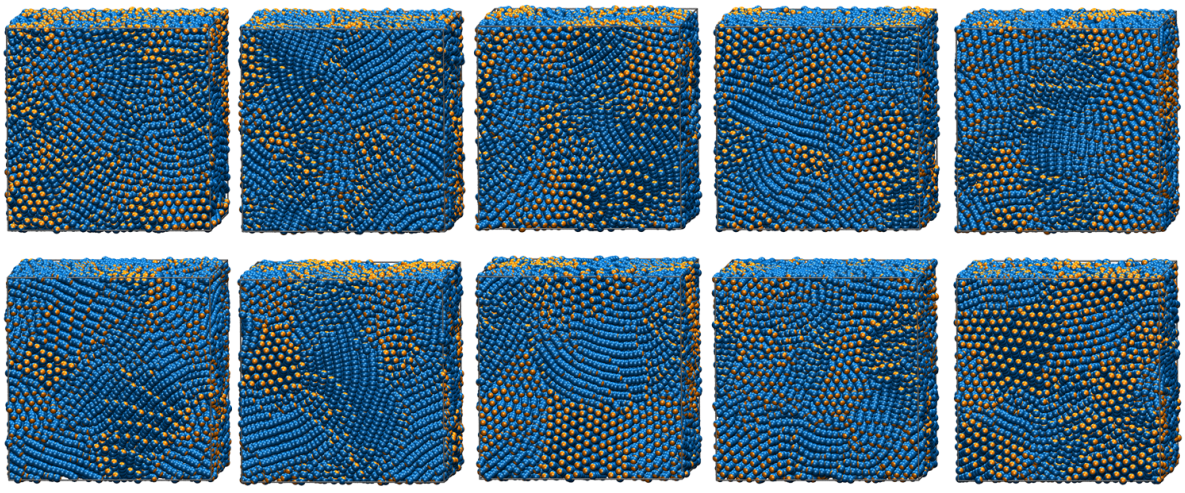

Figure S5: The locally ordered HC packing structures for ten independent simulations with longer time steps (1.6×10^7 time steps) from different initial configurations. In these system, $\alpha_{ij}^{R} = 396$, $\alpha_{ij}^{A} = 176$, $\nu = 0.5$, and $\beta = 45°$.

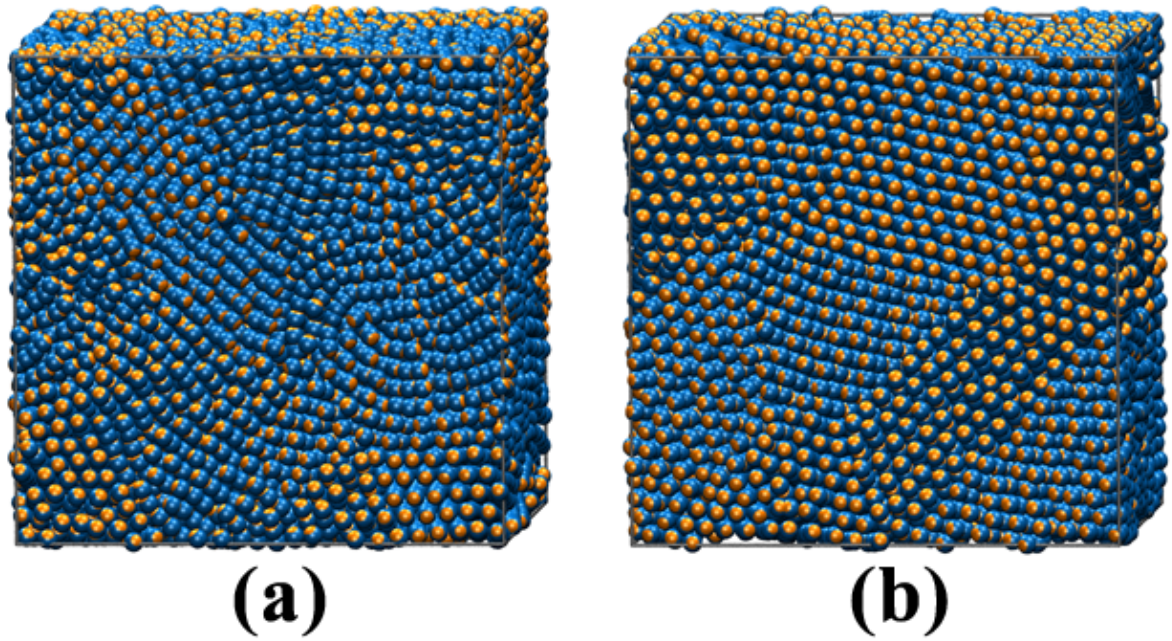

Figure S6: (a) The locally ordered HC packing structure, (b) the more ordered HC packing structure after annealing. The total simulation time is $2.9 \times 10^7 \delta t$, which contains three stages. The first $1.6 \times 10^7 \delta t$ is the relaxation stage at $T = 1.0$. The following $5.0 \times 10^6 \delta t$ is the annealing stage, which contains five annealing cycles. In each cycle, the temperature increases from 1.0 to 2.0 gradually in $5.0 \times 10^5 \delta t$, and then back to 1.0 also in $5.0 \times 10^5 \delta t$. The last $8.0 \times 10^6 \delta t$ is the equilibrium stage at $T = 1.0$ for obtaining the more ordered packing structure. In this system, $\alpha_{ij}^R = 396$, $\alpha_{ij}^A = 176$, $\nu = 0.5$, and $\beta = 45^\circ$.