Supplementary Information: Magnetic-field-induced transitions and phase diagram of aggregate structures in a suspension of polydisperse cubic hematite particles

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I. SIMULATION MOVIES

The simulation video of 2,000,000 MC steps is divided into 200 segments and animated, with each frame representing the state after every 10,000 MC steps. We include the following simulation videos:

1. Movie1.mp4: Generation of initial conditions for σ^*=0.05, σ^*=0.15, σ^*=0.25 and σ^*=0.35.
2. Movie2.mp4: Magnetic field-induced transitions for σ^*=0.05 and λ_0=1.
3. Movie3.mp4: Magnetic field-induced transitions for σ^*=0.05 and λ_0=5.
4. Movie4.mp4: Magnetic field-induced transitions for σ^*=0.05 and λ_0=13.
5. Movie5.mp4: Magnetic field-induced transitions for σ^*=0.35 and λ_0=1.
6. Movie6.mp4: Magnetic field-induced transitions for σ^*=0.35 and λ_0=3.
7. Movie7.mp4: Magnetic field-induced transitions for σ^*=0.35 and λ_0=13.

II. GENERATION OF INITIAL MICROSCOPIC STATES

We employed a microscopic state with randomly arranged and oriented particles as the initial configuration. This state was prepared by initially arranging the particles in a regular pattern and subsequently running 2,000,000 Monte Carlo steps under the conditions $\lambda_0 = 0$ and $\xi_0 = 0$. Figure S1 shows the initial configuration employed in the present study: (a) $\sigma^* = 0.05$, (b) $\sigma^* = 0.15$, (c) $\sigma^* = 0.25$ and (d) $\sigma^* = 0.35$. Simulation movies are provided in Movie1.mp4, showing the simulation process.

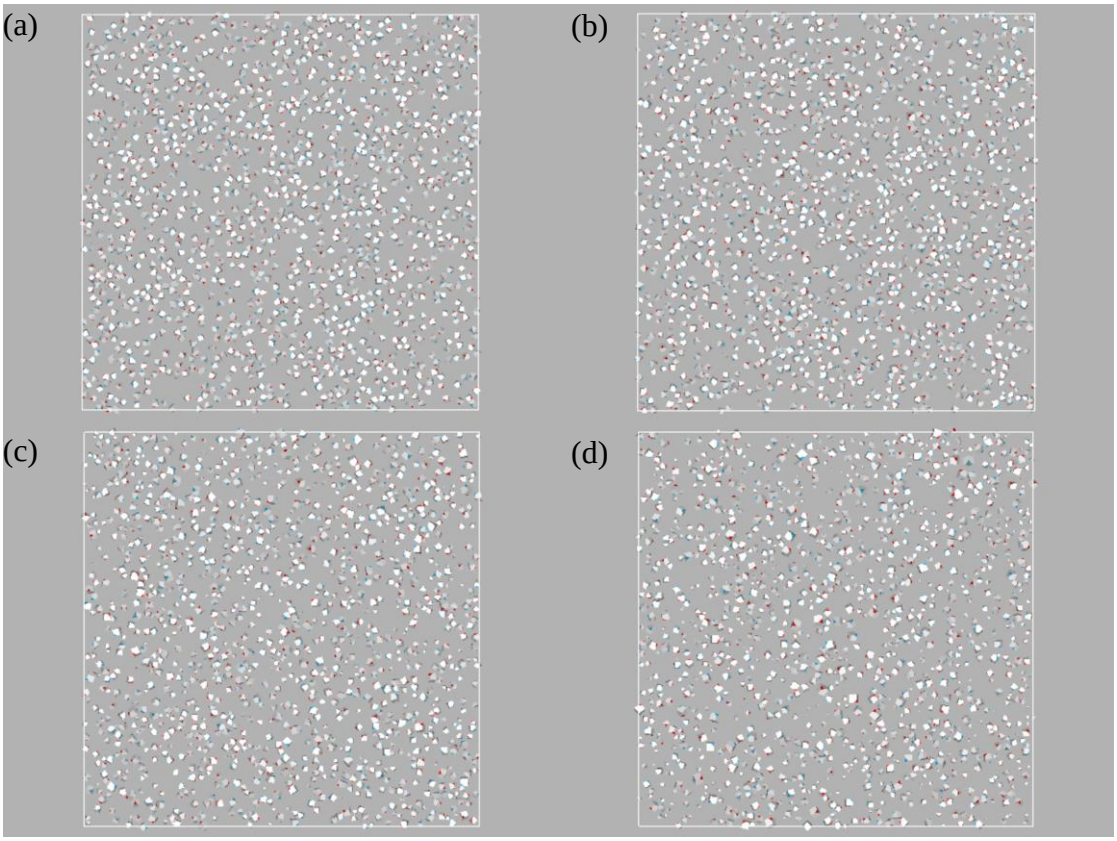

Fig. S1 Initial microscopic states employed in the present study: (a) $\sigma^* = 0.05$, (b) $\sigma^* = 0.15$, (c) $\sigma^* = 0.25$ and (d) $\sigma^* = 0.35$.

III. MAGNETIC FIELD-INDUCED TRANSITIONS

A. For a polydisperse system with a small standard deviation σ^*=0.05

Figure S2 shows particle aggregates for the magnetic particle-particle interaction strength λ_0=1: Figs. S2(a), S2(b), S2(c) and S2(d) are for the cases of the magnetic particle-field interaction strengths ξ_0=1, ξ_0=3, ξ_0=5, ξ_0=15, respectively. Due to the weak magnetic particle-particle interaction, no significant aggregates are formed across all magnetic field regions. The magnetic moments of particles tend to align with the magnetic field direction as the external magnetic field strength increases. Simulation movies are provided in Movie2.mp4, showing the simulation process.

Figure S3 shows particle aggregates for the magnetic particle-particle interaction strength λ_0=5: Figs. S3(a), S3(b), S3(c) and S3(d) are for the cases of the magnetic particle-field interaction strengths ξ_0=1, ξ_0=3, ξ_0=5, ξ_0=15, respectively. Clusters with unstable face-to-face contact and chain-like structures tend to form under varying magnetic field conditions. As the external magnetic field strength increases, chain-like clusters become the dominant structure. Simulation movies are provided in Movie3.mp4, showing the simulation process.

Figure S4 shows particle aggregates for the magnetic particle-particle interaction strength λ_0=13: Figs. S4(a), S4(b), S4(c) and S4(d) are for the cases of the magnetic particle-field interaction strengths ξ_0=1, ξ_0=3, ξ_0=5, ξ_0=15, respectively. As the external magnetic field increases, dense aggregates collapse and transition into thick chain-like clusters aligned along the magnetic field direction. Simulation movies are provided in Movie4.mp4, showing the simulation process.

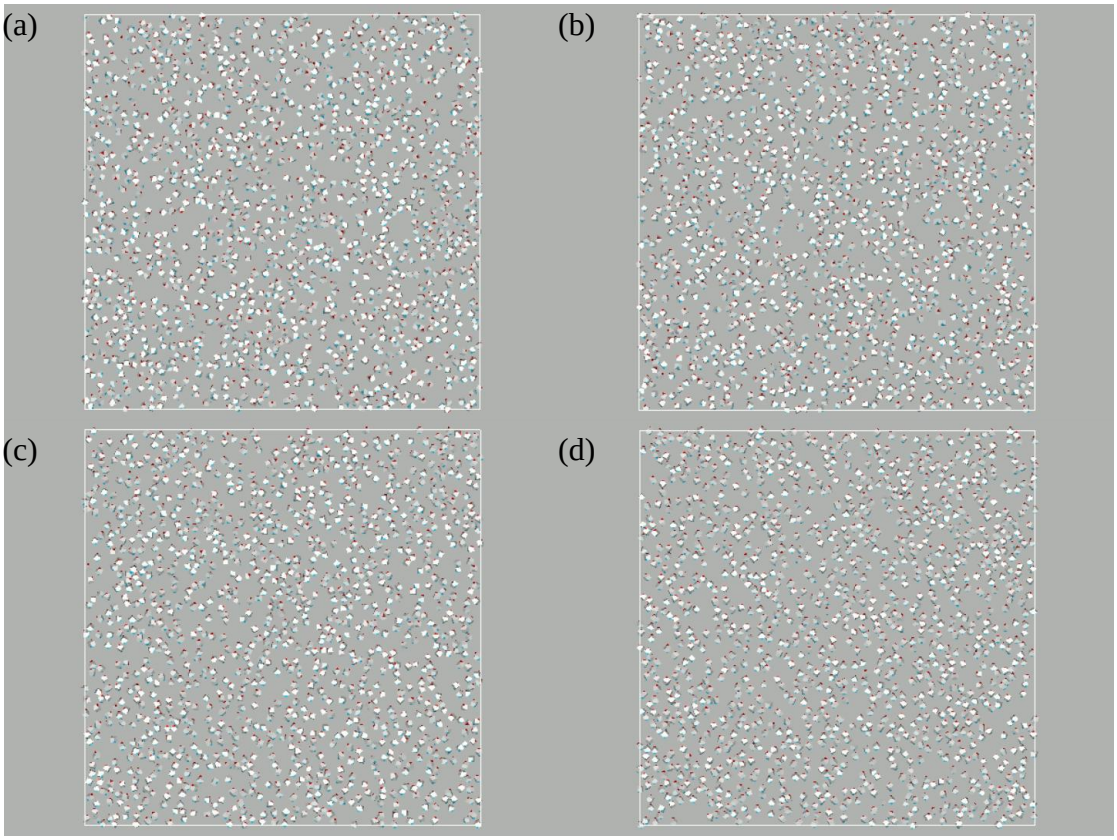

Fig. S2 Magnetic field-induced transitions for σ^*=0.05 and λ_0=1: (a) ξ_0=1, (b) ξ_0=3, (c) ξ_0=5 and (d) ξ_0=15.

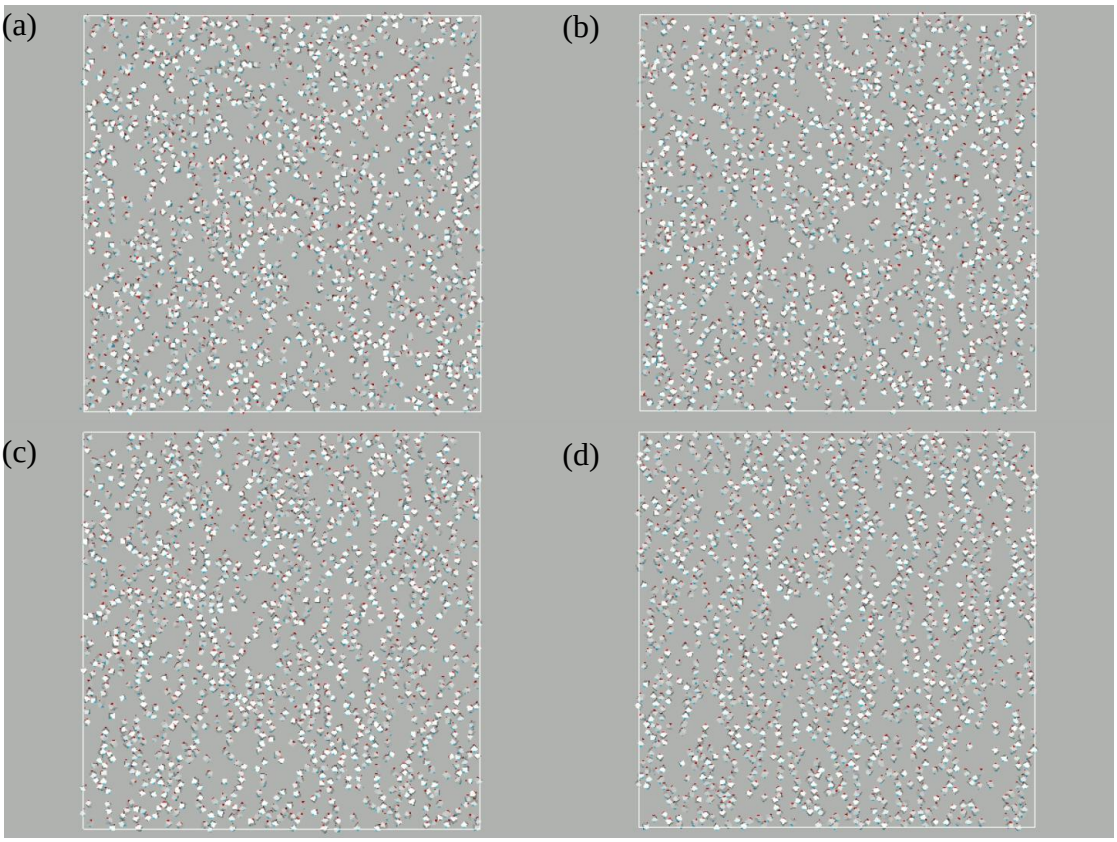

Fig. S3 Magnetic field-induced transitions for σ^*=0.05 and λ_0=5: (a) ξ_0=1, (b) ξ_0=3, (c) ξ_0=5 and (d) ξ_0=15.

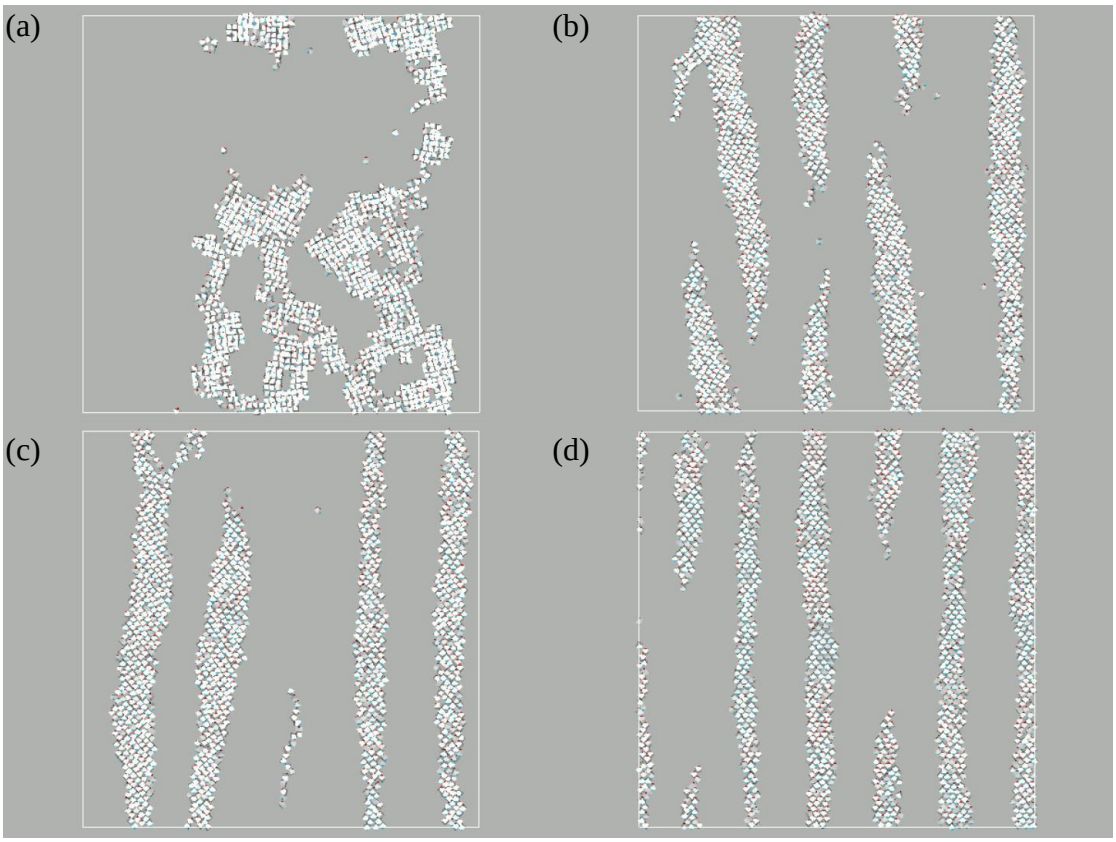

Fig. S4 Magnetic field-induced transitions for σ^*=0.05 and λ_0=13: (a) ξ_0=1, (b) ξ_0=3, (c) ξ_0=5 and (d) ξ_0=15.

B. For a polydisperse system with a large standard deviation σ^*=0.35

Figure S5 shows particle aggregates for the magnetic particle-particle interaction strength λ_0=1: Figs. S5(a), S5(b), S5(c) and S5(d) are for the cases of the magnetic particle-field interaction strengths ξ_0=1, ξ_0=3, ξ_0=5, ξ_0=15, respectively. Due to weak magnetic interactions between particles, most particles in the system exist as single particles. As the strength of the external magnetic field increases, the magnetic moments of the particles gradually align with the field direction. Simulation movies are provided in Movie5.mp4, showing the simulation process.

Figure S6 shows particle aggregates for the magnetic particle-particle interaction strength λ_0=3: Figs. S6(a), S6(b), S6(c) and S6(d) are for the cases of the magnetic particle-field interaction strengths ξ_0=1, ξ_0=3, ξ_0=5, ξ_0=15, respectively. Larger particles aggregate to form network-like clusters and thin chain-like structures. Notably, chain-like clusters tend to grow larger as the strength of the external magnetic field increases. Simulation movies are provided in Movie6.mp4, showing the simulation process.

Figure S7 shows particle aggregates for the magnetic particle-particle interaction strength λ_0=13: Figs. S7(a), S7(b), S7(c) and S7(d) are for the cases of the magnetic particle-field interaction strengths ξ_0=1, ξ_0=3, ξ_0=5, ξ_0=15, respectively. Strong magnetic particle-particle interactions lead to the formation of dense aggregates. As the external magnetic field increases, these aggregates transition into thick chain-like clusters through intermediate complex structures. Simulation movies are provided in Movie7.mp4, showing the simulation process.

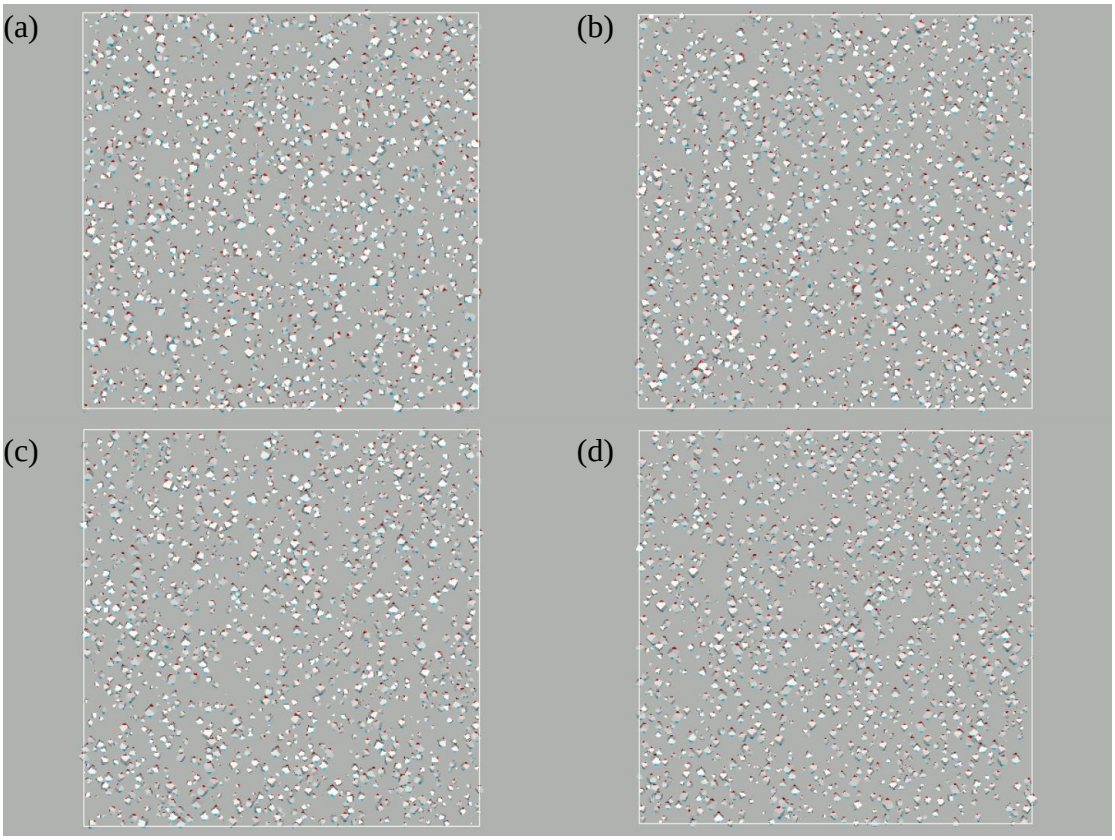

Fig. S5 Magnetic field-induced transitions for σ^*=0.35 and λ_0=1: (a) ξ_0=1, (b) ξ_0=3, (c) ξ_0=5 and (d) ξ_0=15.

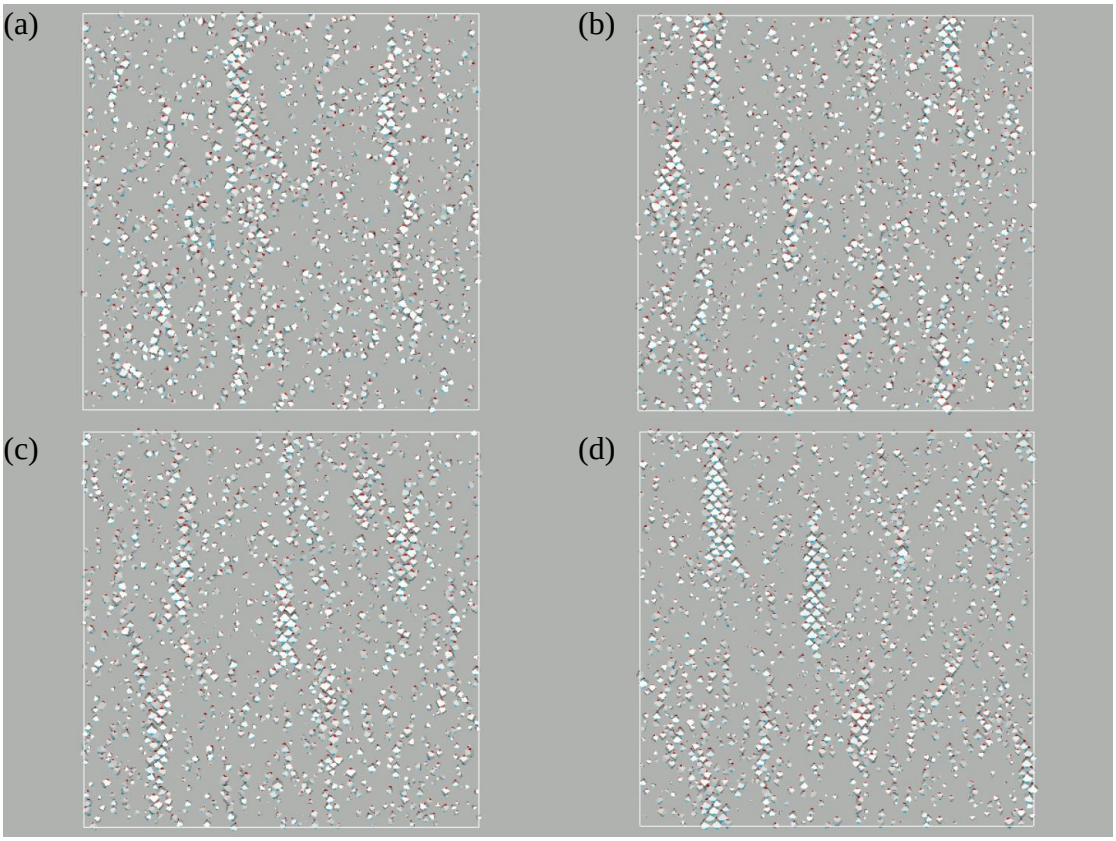

Fig. S6 Magnetic field-induced transitions for σ^*=0.35 and λ_0=3: (a) ξ_0=1, (b) ξ_0=3, (c) ξ_0=5 and (d) ξ_0=15.

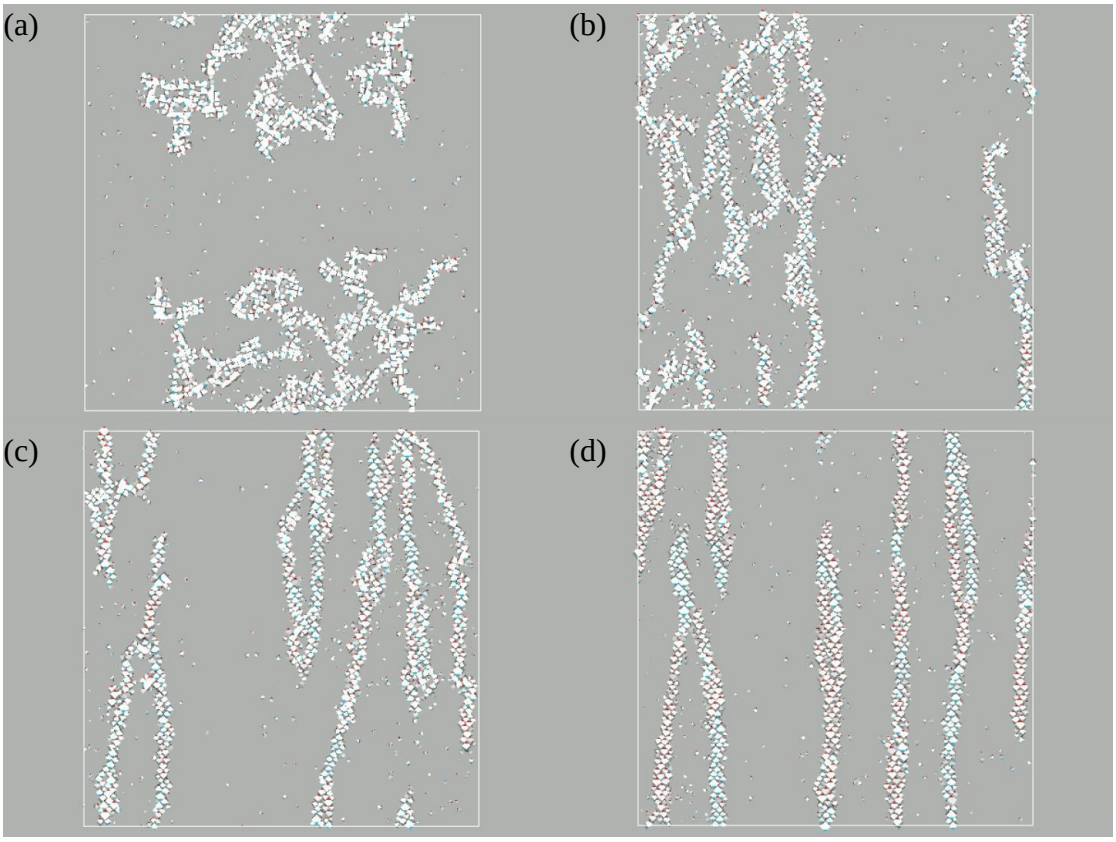

Fig. S7 Magnetic field-induced transitions for σ^*=0.35 and λ_0=13: (a) ξ_0=1, (b) ξ_0=3, (c) ξ_0=5 and (d) ξ_0=15.