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How Magnetic Moment Angle Governs Self-Assembly and Aggregation Kinetics of Cubic Hematite Particles in a Quasi-Two-Dimensional System

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Cubic hematite particles can form different kinds of aggregate structures, but the effect of the magnetic moment angle has not been studied systematically. In this study, we examined a quasi-two-dimensional system, where the particle centers were confined to a plane, while the particles were still free to rotate in three dimensions. Monte Carlo simulations were used to study equilibrium structures, and Brownian dynamics simulations were used to follow the aggregation process from dispersed states. First, we compared three typical magnetic moment directions: face-normal, edge, and body-diagonal. The face-normal case mainly formed chain-like clusters, while the edge and body-diagonal cases formed denser clusters with frequent face-to-face contacts. Next, we changed the magnetic moment direction continuously around the body-diagonal direction to see how the aggregate structures changed. A clear difference was found between the two sides. When the magnetic moment direction was changed from the body-diagonal direction toward the face-normal direction, the structures changed from closely packed clusters to ring-like and then chain-like clusters. This change became especially clear around 15° to 20°. In contrast, when the direction was changed toward the edge direction, the structural changes were small. The Brownian dynamics results also showed that the aggregation process strongly depends on the stability of small clusters formed at the early stage. These results suggest that even a small change in the magnetic moment angle can strongly affect both the aggregate structures and the aggregation process.

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