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Insights into the energy landscape of janus and triblock magnetic particles

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Understanding the self-assembly of patchy magnetic particles requires a detailed characterization of their anisotropic interaction landscapes. While molecular dynamics simulations reveal a rich variety of assembled structures, extending beyond the conventional formation of chains and rings 1, a complementary theoretical framework is necessary to rationalize their stability and competition.

To this end, we employ a one-parameter rotational pathway that continuously connects highly symmetric configurations at fixed interparticle distance, inspired by Brillouin-zone sampling in crystalline systems. This representation, recently introduced for charged patchy particles [2], enables a compact and systematic mapping of the interaction energy as a function of relative particle orientation and is applicable to both dipolar (Janus) and quadrupolar (triblock) symmetries.

Using this framework, we analyze how shifting the magnetic patches modifies the energy landscape. In the triblock case, we identify three dominant configurations—parallel, antiparallel and orthogonal – that govern the interaction behavior. Increasing the patch shift induces a nontrivial competition between these states, enhancing configurational diversity and promoting the emergence of complex assemblies. In the Janus case, the same representation captures the established competition between parallel and antiparallel configurations [3], while providing additional insight into the structure of the energy landscape along continuous rotational paths.

These findings provide a new perspective on the role of anisotropy in magnetic patchy particles and offer design tools for tuning self-assembly through controlled modifications of particle geometry and interaction symmetry.

References

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