Coarse-Grained Contact-Area Dominated Interaction for Two-Dimensional Colloidal Nanoparticles

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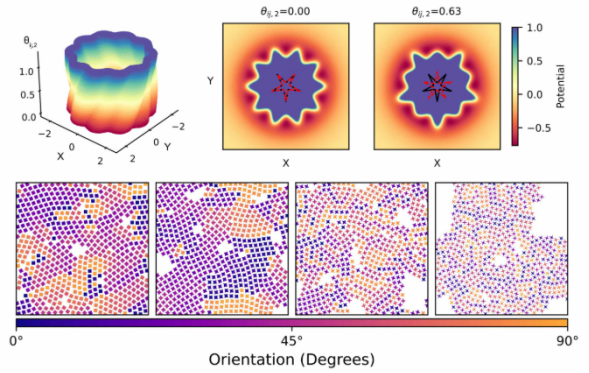
The self-assembly of anisotropic nanoparticles offers a versatile route to designing materials with tunable optical and mechanical properties [1-3]. However, a significant body of research relies on the hard-particle model [4], which often fails to capture the essential physics of ligand-stabilized colloids. We present a coarse-grained interaction model that bridges this gap by explicitly accounting for the "softness" and contact-area dependence of the ligand shell. Unlike computationally expensive atomistic summations, our method derives an effective pair potential using a Derjaguin-like approximation [5]. This approach allows us to tune the ligand length while ensuring interactions scale correctly with the contact area of arbitrary shapes. By integrating this potential over particle boundaries, we generate tabulated energy landscapes that enable efficient 2D Molecular Dynamics (MD) simulations of arbitrary geometries. We also derive an analytical form of this interaction energy. We demonstrate that introducing shell softness alters the phase diagram, revealing a competition between core anisotropy and ligand-mediated interactions. This framework offers a physically grounded yet computationally efficient tool for predicting the assembly of realistic colloidal nanoparticles.

Keywords:
Anisotropic colloidal nanoparticles modeling, coarse-grained interactions, two-dimensional systems, self-assembly, MD simulations



Visualization of the interaction potential in different spaces and the snapshots of the resulting assemblies.

References:

[1] Zhong, Y. et al. Nat Chem Eng 1, 532–541 (2024).
[2] Murphy, C. J. et al. J. Phys. Chem. B 109, 13857–13870 (2005).
[3] Xia, Y., Chen, Q. & Banin, U. Chem. Rev. 123, 3325–3328 (2023).
[4] Damasceno, P.F., Engel, M., Glotzer, S.C., Science 337, 453–457 (2012).
[5] Derjaguin, B. Kolloid-Zeitschrift 69, 155–164 (1934).

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