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Binding, Curvature-Sensing, Curvature-Generation and Self-Assembly of Anisotropically Curved Nanoparticles on Lipid Membranes

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Golgi and endoplasmic reticulum in eukaryotic cells, owe their complex membrane conformations to specialized proteins known as BAR domains. Using coarse-grained molecular dynamics simulations [1], we investigated the binding and aggregation of anisotropically curved nanoparticles (NPs), akin to BAR domains, to tubular and spherical lipid vesicles. The ability of a NP to bind to a tubular membrane depends on the NP-lipid interaction strength, mismatch between the curvature of the NP and the tubular membrane, and the N's arclength. We found that the minimum interaction strength required for a NP binding increases with increasing the mismatch between the curvatures of the NP and the tubular membrane or increasing the NP arclength. We also investigated the aggregation of these NPs on lipid vesicles and found that they self-assemble into chains or asters depending on the NPs curvature and NP-lipid interaction strength. In particular, chains form for low NP-curvature or NP-lipid interaction strength, while asters form for high NP-curvature or high NP-lipid interaction strength [1] M. Laradji, P.B. Sunil Kumar, and E.J. Spangler, J. Phys. D: Appl. Phys. **49**, 293001 (2016)

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