Cell Responses to Actively Rotational Nanoparticles: A Coarse-Grained Study

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Understanding and controlling the interaction of actively rotational nanoparticle (RNP) with cell is critical to the development of its biomedical applications. Here we perform dissipative particle dynamics simulations to analyze the rotation period, size, and coating pattern as RNP interacts with the cell so as to provide novel design of drug delivery applications. It has shown that the actively RNP is capable to intriguer local disturbance and promotes the cell translocation toward RNP. During the studies, we mainly focused on the translocation time required for RNP entering inside cell under various rotation periods as well as the interaction energy between coated RNP and cell. Through ligand pattern design on RNP, we could find a suitable nanoparticle candidate with a specific ligand coating pattern for drug delivery. We also find that channel-like RNP could connect the cells to form the network which facilitate the substances change between the cells. Our findings provide useful guidelines for the molecular design of patterned RNP for controllable interfaces and help establish qualitative rules for the organization and optimization of ligands for desired drug delivery.

Keywords: Nanoparticle, Cell membrane, Drug delivery, Dissipative Particle Dynamics