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Interaction of Biofunctionalized Nanoparticles with Receptors on Cell Surfaces: MC Simulations ELENA DORMIDONTOVA, Physics Department and Institute of Materials Science, University of Connecticut, SHIHU WANG, Chemical Engineering Department, University of Michigan — One of the areas of active development of modern nanomedicine is drug/gene delivery and imaging application of nanoparticles functionalized by ligands, aptamers or antibodies capable of specific interactions with cell surface receptors. Being a complex multifunctional system different structural aspects of nanoparticles affect their interactions with cell surfaces and the surface properties of cells can be different (e.g. density, distribution and mobility of receptors). Computer simulations allow a systematic investigation of the influence of multiple factors and provide a unified platform for the comparison. Using Monte Carlo simulations we investigate the influence of the nanoparticle properties (nanoparticle size, polymer tether length, polydispersity, density, ligand energy, valence and density) on nanoparticle-cell surface interactions and make predictions regarding favorable nanoparticle design for achieving multiple ligand-receptor binding. We will also discuss the implications of nanoparticle design on the selectivity of attachment to cells with high receptor density while “ignoring” cells with a low density of receptors.

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