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Design of Polymer-Grafted Particles for Biocompatability DAVID TROMBLY, VENKAT GANESAN, Department of Chemical Engineering, University of Texas at Austin — Drug designers often coat drug particles with grafted polymers in order to introduce a net repulsion between the particles and blood proteins. This net repulsion results from the energy cost of compressing grafted chains on approach of proteins. It thus overcomes the Van Der Waals attraction between drug and protein which would otherwise cause particle-protein agglomeration and ultimately thrombosis. This study proposes to develop a fundamental understanding of the role of different features in controlling the efficacy of the grafted layers. We address this issue by developing a framework to predict the interactions between a polymer-coated spherical particle and a bare spherical particle. In order to fully capture the two-sphere system, a numerical solution of polymer mean field theory is used in a bispherical coordinate system. Results for protein-particle interaction energies for different design parameters will be presented. For biological applications, polyethylene glycol is often used as the grafted polymer. The unique properties of this molecule will be accounted for using the n-cluster model.

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