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Thermodynamic analysis of multivalent binding of functionalized nanoparticles to the cell membrane surface SAMANEH FAROKHIRAD, New Jersey Institute of Technology, RYAN BRADLEY, RAVI RADHAKRISHNAN, University of Pennsylvania — h $-abstract-$\pardWe present a quantitative model for multivalent binding of ligand-coated flexible polymeric nanoparticles (NPs) to a membrane expressing receptors. The model is developed using a multiscale computational framework by coupling a continuum field model for the cell membrane with a coarse-grained model for the NP. The NP is modeled as a bead-spring polymer chain, and the membrane is modeled as a dynamically triangulated surface. The NP binding affinity to a cell surface is mainly determined by the delicate balance between the enthalpic gain due to the ligand-receptor binding and the entropic penalties of various components. We show that the multivalent interactions between the NP and the cell surface are subject to entropy-enthalpy compensation. Three different entropy contributions, namely, those due to receptor-ligand translation, NP flexibility, and membrane undulations, are all significant, although the first of these terms is the most dominant. However, both NP flexibility and membrane undulations dictate the receptor-ligand translational entropy making the entropy compensation context-specific,i.e., dependent on whether the NP is rigid or flexible, and on the state of the membrane. \pard-/abstract-\

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