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Designing super-selectivity in multivalent nano-particle binding¹ FRANCISCO MARTINEZ-VERACOECHEA, DAAN FRENKEL, University of Cambridge — A key challenge in nano-science is to design ligand-coated nanoparticles that can bind selectively to surfaces that display the cognate receptors above a threshold (surface) concentration. Nano-particles that bind monovalently to a target surface do not discriminate sharply between surfaces with high and low receptor coverage. In contrast, "multivalent" nano-particles that can bind to a larger number of ligands simultaneously, display regimes of "super-selectivity" where the fraction of bound particles varies sharply with the receptor concentration. We present numerical simulations that show that multivalent nano-particles can be designed such that they approach the "on-off" binding behavior ideal for receptorconcentration selective targeting. We propose a simple analytical model that accounts for the super-selective behavior of multi-valent nano-particles. We propose a simple rule of thumb to predict the conditions under which super-selectivity can be achieved. We validate our model predictions against the Monte Carlo simulations. Finally, we investigate the role of multi-component ligand-receptor interactions in the enhancement of targeting selectivity.

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