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Mean-Field Modeling of the Encapsulation of Weakly Acidic Particles in Polyelectrolyte Dendrimers THOMAS LEWIS, VENKAT GANESAN, University of Texas at Austin — The unique architecture of dendrimers has attracted interest in a wide-variety of biomedical applications such as drug delivery. Dendrimers act as covalent micelles and have been shown experimentally to internalize hydrophobic molecules inside their cavities. Moreover, many drugs of low water solubility are weakly acidic and have been shown to form complexes with polybasic dendrimers, with the encapsulation ability being dependent upon the solution pH. Furthermore, the grafting of neutral water soluble chains such as polyethylene glycol (PEG) have shown to increase the encapsulation of poorly soluble drug molecules. In order to gain insight into the equilibrium behavior of drug-dendrimer complexes, we have developed and numerically solved a Self-Consistent Field Theory approach for both grafted and non-grafted annealed charged dendrimer molecules in the presences of drug molecules. Specifically, this work examines the effect of drug size, dendrimer generation, grafting chain length, and solution pH upon dendrimer encapsulation abilities.

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