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Structural and phase transitions of one and two polymer mushrooms DELIAN YANG, QIANG (DAVID) WANG, Colorado State University — A polymer mushroom here refers to a group of n homopolymer chains end-grafted at the same point on a flat, impenetrable and homogeneous substrate. Using lattice self-consistent field (LSCF) calculations with the Kronecker δ-function interactions (instead of the commonly used nearest-neighbor interactions), we have studied the structures of one and two polymer mushrooms in an explicit solvent as a function of the polymer volume fraction, the solvent quality characterized by the Flory-Huggins χ parameter, and the distance between the two mushrooms. We have constructed phase diagrams of these systems showing the coil-globule transition (CGT) of one mushroom and how it is coupled with the fused-separated transition (FST) of two mushrooms. Since LSCF results are exact only in the limit of $n \to \infty$, we also use the newly proposed fast lattice Monte Carlo (FLMC) simulations[1] with the same Hamiltonian as in LSCF theory to examine how this limit is approached with increasing n. Direct comparisons between LSCF and FLMC results without any parameter-fitting quantify the fluctuation/correlation effects neglected in LSCF theory. We also find a second-order symmetric-asymmetric transition (SAT) for one-mushroom system in the globule state, and examine its coupling with CGT and FST. [1] *Q. Wang*, **Soft Matter, 5**, 4564 (2009); **6**, 6206 (2010).

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