Abstract Submitted
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Solvent Repacking Monte Carlo: Application to Phase Behavior of Hard-Disk Mixtures JAMES KINDT, Emory University — An adaptation of configuration bias Monte Carlo called Solvent Repacking Monte Carlo has been developed for grand canonical MC simulation of solutes in condensed phase solutions. This algorithm enables the insertion or removal of a large solute in exchange for a variable number of solvent molecules, which are removed to make room for the solute or "repacked" into the solute's cavity. For a proof of concept it has been applied to hard disk mixtures, where the "solutes" are disks of radius between 1.4 and 3 times greater than the solvents. The method is efficient enough to allow for the equilibration of the number and spatial distribution of large disks embedded among small disks even above the freezing transition, and allows the estimation of phase boundaries and compositions at coexistence of the fluid and ordered phases in binary hard disk mixtures. The partitioning of large disks between the phases varies non-monotonically with diameter ratio. Possibilities for the applicability of the method to simulations of aqueous solutions using atomistic models will be discussed.

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