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Solvent Evaporation Induced Assembly in Binary Mixtures of Nanoparticles[1] SHENGFENG CHENG, YANFEI TANG, Virginia Polytechnic Institute and State University, GARY GREST, Sandia National Laboratories — Large-scale molecular dynamics simulations are used to study the ordering induced by evaporating the solvent from a solution containing nanoparticles of two different sizes. A thick fluid film containing the solvent and nanoparticles in contact with the solvent vapor is first equilibrated. In this initial state there is an excess of the smaller nanoparticles near the liquid/vapor interface. The solvent evaporation process is initiated by removing the vapor at a controlled rate from a region far from the interface. Our results show that the ordering of nanoparticles is determined by the competition between the evaporation-induced movement of the liquid/vapor interface and the diffusion of the nanoparticles, which can be characterized by a dimensionless Peclet (Pe) number for each type of nanoparticles. When $Pe \gg 1$ for both nanoparticles, the accumulation of the smaller nanoparticles near the interface is enhanced during evaporation. However, when $Pe > 1$ for the larger nanoparticles while $Pe < 1$ for the smaller ones, the ordering exhibits the opposite trend with the larger nanoparticles accumulating near the interface. Our results reveal the critical role of the evaporation rate of the solvent on controlling the distribution of nanoparticles.

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