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Interfacial free energy calculation of a binary hard-sphere fluid at a hard wall by Gibbs-Cahn Integration JESSE KERN, BRIAN LAIRD, University of Kansas — The interfacial free energy, γ, of fluids at surfaces is a parameter that is central to a number of technologically important phenomena, such as wetting, nucleation and the stability and self assembly of colloidal particles in solution. In recent years, our group has developed techniques to determine γ from atomistic simulation. In this work, we apply one of these methods, Gibbs-Cahn Integration, to determine γ for a model two-component (binary) mixture of hard spheres. Molecular dynamics simulation is used to characterize a hard-sphere fluid mixture in a slit-pore confined geometry as packing fraction, mole fraction, and diameter ratio are varied. We find that recent theoretical predictions from the White Bear II classical density functional theory [Roth et al., J. Phys.: Condens. Matter, *18*, 8413, (2006)] agree well with our computational results We also observe that, for this model system, the preferential adsorption of one particle species over the other contributes negligibly to the interfacial free energy at modest diameter ratios.

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