

Vapor-liquid phase equilibria for linear and branched alkane monolayers physisorbed on Au(111)

Jeffrey J. Potoff^{1,2*} and J. Ilja Siepmann^{1†}

¹*Departments of Chemistry and of Chemical Engineering and Materials Science,
University of Minnesota, Minneapolis, MN 55455-0431*

²*Department of Chemical Engineering and Materials Science,
Wayne State University, Detroit, MI 48202*

Abstract

Histogram-reweighting Monte Carlo simulations in the grand canonical ensemble were used to obtain vapor-liquid coexistence curves for a series of alkanes physisorbed on a flat gold substrate. The critical temperatures and densities of *n*-alkanes from methane to decane as well as the branched molecules 2-methylpropane, 2,2-dimethylbutane and 2,3-dimethylbutane were determined through a mixed-field analysis. The ratio of the 2D (two-dimensional) to the 3D (three-dimensional) critical temperature was found to depend weakly on the chain length for *n*-alkanes, decreasing from $T_c^{2D}/T_c^{3D} = 0.38$ for methane to $T_c^{2D}/T_c^{3D} = 0.31$ for *n*-decane. In contrast to typical bulk fluid behavior, the branched isomers were found to have higher critical temperatures than their linear counterparts.

*Present address: Wayne State University

†To whom correspondence should be addressed. E-mail: siepmann@chem.umn.edu.