

Abstract Submitted  
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**Size-dependent segregation, separation, and ordering in an alkane mixture undergoing slow compression in a confining narrow gap**<sup>1</sup> LINA MERCHAN, JIANPING GAO, UZI LANDMAN, School of Physics, Georgia Institute of Technology — With the use of grand-canonical molecular dynamics simulations, we studied the slow compression (0.01m/s) of liquid films made of pure hexane and hexadecane, and of an equimolar mixture of the two alkanes, confined between two opposing crystalline gold surfaces. The organization of the density of the confined films into layered structures, intra-layer ordering in the interfacial layers, orientational order parameters, diffusion coefficients, and force versus gap-size profiles, recorded during slow compressions of the above systems, are analyzed and compared. The longer chain molecule preferentially adsorb to the solid surfaces, resulting in size-induced segregation near the solid-liquid interfaces. As a result, the slow compression (reducing the gap-size,  $d$ ) causes preferential separation of the hexadecane/hexane mixture, from 50:50 at  $d = 3.6$  nm to 80:20 at  $d = 1.7$  nm, with the longer chains of the hexadecane molecules crystallizing into ordered layers between the opposing gold surfaces.

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