

Abstract Submitted  
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**Continuum Mean-Field Theories for Molecular Fluids, and Their Validity at the Nanoscale**<sup>1</sup> C.B. HANNA, Boise State University, F. PEYRONEL, University of Guelph, C. MACDOUGALL, St. Francis Xavier University, A. MARANGONI, University of Guelph, D.A. PINK, St. Francis Xavier University, AFMNET-NCE COLLABORATION — We present a calculation of the physical properties of solid triglyceride particles dispersed in an oil phase, using atomic-scale molecular dynamics. Significant equilibrium density oscillations in the oil appear when the interparticle distance,  $d$ , becomes sufficiently small, with a global minimum in the free energy found at  $d \approx 1.4$  nm. We compare the simulation values of the Hamaker coefficient with those of models which assume that the oil is a homogeneous continuum: (i) Lifshitz theory, (ii) the Fractal Model, and (iii) a Lennard-Jones 6-12 potential model. The last-named yields a minimum in the free energy at  $d \approx 0.26$  nm. We conclude that, at the nanoscale, continuum Lifshitz theory and other continuum mean-field theories based on the assumption of homogeneous fluid density can lead to erroneous conclusions.

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