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Capillary waves at the water liquid-vapor interface AHMED E. ISMAIL, GARY S. GREY, MARK J. STEVENS, Sandia National Laboratories — Evidence for capillary waves at the liquid-vapor interface of water is presented from molecular dynamics simulations. The total interfacial width includes a correction term which depends logarithmically on the length L_{\parallel} of the simulation cell parallel to the interface, and which is inversely proportional to the surface tension γ_{cw} . Comparison of γ_{cw} for system sizes up to 10^5 molecules to γ_p , obtained from the difference between the pressure parallel and the pressure perpendicular to the interface, yields adequate agreement only if one fits the interfacial profile to an error function and not to a hyperbolic tangent, as often assumed. Results for γ for a number of atomistic three-site (SPC/E, TIP3P, TIP3P-CHARMM, and TIP3P-Ew) and four-site (TIP4P and TIP4P-Ew) non-polarizable water models are compared to experiment for temperatures from 300 K to 500 K, and for a variety of interaction cutoffs and reciprocal-space mesh refinements. Our results show that the SPC/E model is more accurate than the other available three-site models, while the original TIP3P model is closer to experimental data than its more recent parameterizations.

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