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Molecular Modeling of Three Phase Contact for Static and Dynamic Contact Angle Phenomena ATEEQUE MALANI, Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, MIGUEL AMAT, Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ, ANILKUMAR RAGHAVANPILLAI, E.I. du Pont de Nemours,, Wilmington, DE, ERNEST WYSONG, Experimental Section, E.I. du Pont de Nemours,, Wilmington, DE, GREGORY RUTLEDGE, Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA — Interfacial phenomena arise in a number of industrially important situations, such as repellency of liquids on surfaces, condensation, etc. In designing materials for such applications, the key component is their wetting behavior, which is characterized by three-phase static and dynamic contact angle phenomena. Molecular modeling has the potential to provide basic insight into the detailed picture of the three-phase contact line resolved on the sub-nanometer scale which is essential for the success of these materials. We have proposed a computational strategy to study three-phase contact phenomena, where buoyancy of a solid rod or particle is studied in a planar liquid film. The contact angle is readily evaluated by measuring the position of solid and liquid interfaces. As proof of concept, the methodology has been validated extensively using a simple Lennard-Jones (LJ) fluid in contact with an LJ surface. In the dynamic contact angle analysis, the evolution of contact angle as a function of force applied to the rod or particle is characterized by the pinning and slipping of the three phase contact line. Ultimately, complete wetting or de-wetting is observed, allowing molecular level characterization of the contact angle hysteresis.

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