Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

First principles Modelling of Brush formation of linear oligomers on Al Surfaces COLIN DENNISTON, LINGTI KONG, University of Western Ontario, MARTIN MUESER, Universitat des Saarlandes — We study the role of chemical detail in short-linear parafins and olefins in the formation of polymer brushes on an Aluminum substrate. The presence of unsaturated bonds near the end of the chain greatly enhances the brush formation on the Al surface. In addition we examine the resulting change in slip boundary conditions for flow over the surface. Our simulations are based on a molecular dynamics force field we have developed using force matching to density functional theory with careful attention to correct reproduction of lateral as well as normal forces.

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Date submitted: 20 Nov 2009 Electronic form version 1.4