Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Molecular dynamics simulations of dotriacontane films supported on a SiO_2 surface SEBASTIAN GUTIERREZ, Pontificia Universidad Catolica de Chile, RAUL ARAYA, TOMAS PEREZ-ACLE, Universidad de Chile, MARIA JOSE RETAMAL, ULRICH G. VOLKMANN, Pontificia Universidad Catolica de Chile — Dotriacontane ($C_{32}H_{66}$, C32) films supported on SiO_2 surfaces were studied using very high-resolution ellipsometry, atomic force microscopy (AFM) and x-ray reflectivity techniques. For almost complete layers a model was proposed [1] in which the C32/SiO_2 interfacial region is characterized by a parallel bilayer and perpendicular layers on top. Recent AFM measurements performed on samples forming sea-weed like structures, showed that for these particular perpendicular "fractal like" layers the heights are lower than the all-trans length of dotriacontane (42.5 Å). To gain insights on the internal molecular ordering and layering of C32 supported on SiO_2 surfaces, we used all-atom molecular dynamics to simulate C32 films at different temperatures. Our results confirm the presence of the parallel bilayer suggesting the existence of a mixed layer on top, formed by molecules with both parallel and perpendicular segments. These findings suggest a different molecular architecture for sea-weed like structures of dotriacontane supported on SiO_2.

[1] H. Mo et al., Chem. Phys. Lett. **377**, 99-105 (2003); U. G. Volkmann, et al., J. Chem. Phys. **116**, 2107 (2002).

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Date submitted: 30 Dec 2010 Electronic form version 1.4