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$_2$.