

Supplementary Information.

In situ study of alkane phosphate film formation and stability on TiO₂

Stephen A. Holt*^a Anton P. Le Brun^a Andrew R.J. Nelson^a and J.H. Lakey

Table S1. Calculated SLD values, assuming Headgroup and Tail molecular volumes of 213.78 and 59.55 Å³ respectively.

Material	SLD (x 10 ⁻⁶ Å ⁻²)
Silicon	2.07
Silicon Oxide	3.47
Titanium Oxide	2.36
Phosphate Headgroup	4.76
Dodecyl Tail	-0.622
H ₂ O	-0.55
D ₂ O	6.35

Below are figures summarising the data and fitting from the NR pH series experiments. In all cases only D₂O buffer datasets have been shown. Data was recorded for each step in the pH range from 4.5 to 9.5 was with D₂O and/or TiO₂M subphases. In Figure S1 at pH 4.5 data washed was only collected with a TiO₂M subphase hence there is no dataset on the figure. Similarly for the pH 7.0 preparation series there is no D₂O dataset a pH 5.5.

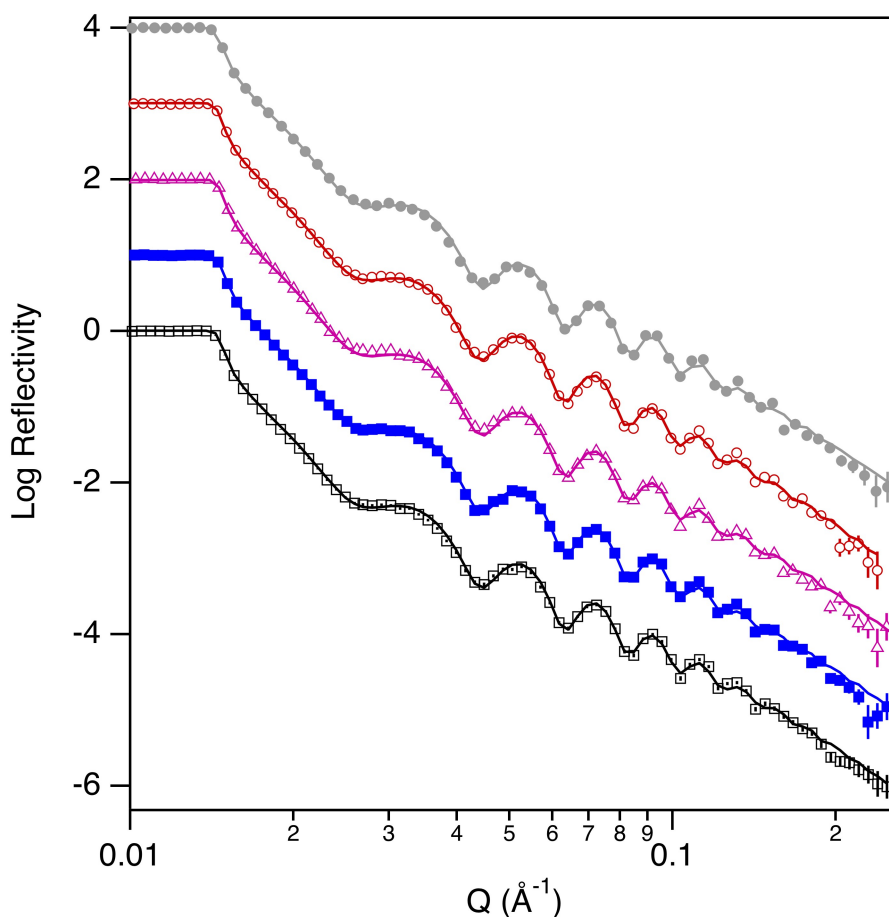


Figure S1a. NR data (symbols) and fits (lines) for a dodecyl phosphate film prepared at pH 4.5 with an incubation time of 1140 minutes. Black – pH 5.5; Blue – pH 6.5; Magenta – pH 7.5; Red – pH 8.5, Grey – pH 9.5.

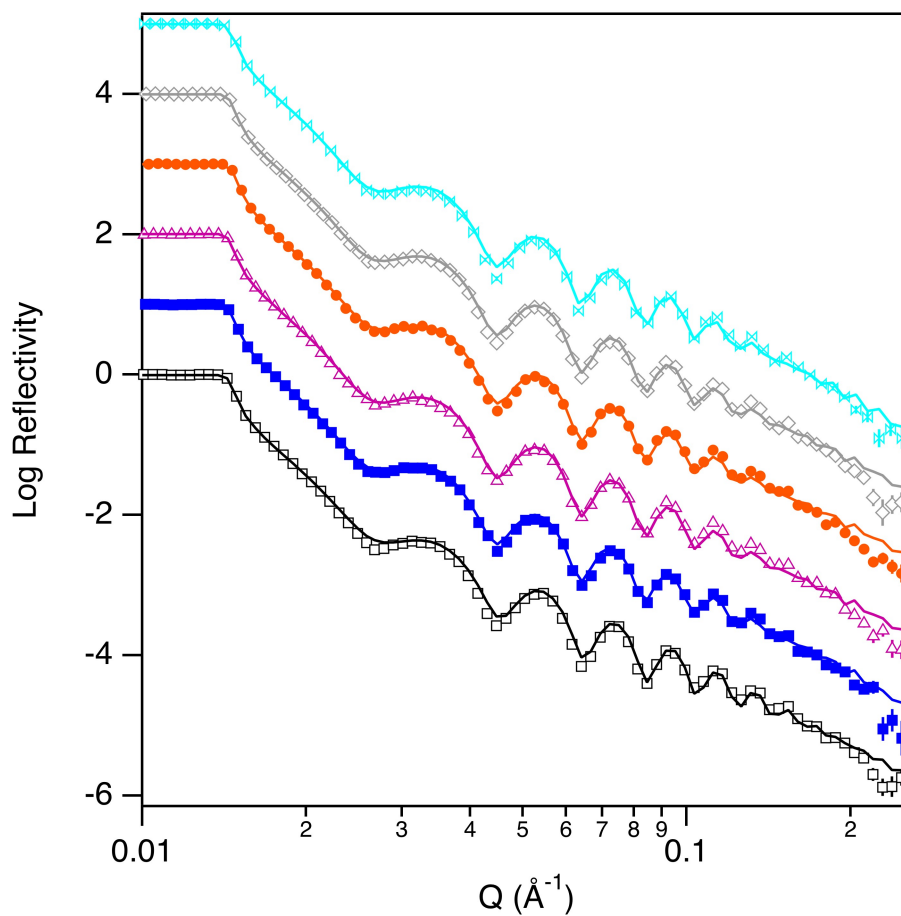


Figure S1b. NR data (symbols) and fits (lines) for a dodecyl phosphate film prepared at pH 7.0 with an incubation time of 1020 minutes. Black – pH 7.0; Blue – pH 4.5; Magenta – pH 6.5; Red – pH 7.5, Grey – pH 8.5; Cyan – pH 9.5.