# First Principles Modelling of Growth of Hybrid Organic-Inorganic Films

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Organic-inorganic hybrid materials are a unique class of materials with unique properties which means they are useful in flexibile devices. Molecular layer deposition (MLD) offers novel pathways for the fabrication of such hybrids by using metallic precursors and a vast range of organic precursors. To investigate and understand the mechanism of growth and stability a combination of theoretical and experimental data is needed.

In this contribution, we present a first principles investigation of the molecular mechanism of the growth of hybrid organic−inorganic thin films of aluminium alkoxides, known as ”alucones” grown by MLD. We focus on the interactions between precursors and this is explored by analyzing the MLD reaction products between the post-TMA Monomethyl-$Al_2O_3$ (Al-$CH_3$-$Al_2O_3$) and Dimethyl-$Al_2O_3$ (Al$(CH_3)_2$-$Al_2O_3$) surface and the organic precursors ethylene glycol (EG), diethylene glycol (DEG), triethylene glycol (TEG) and tetraethylene glycol (FEG). The energetics of the reaction of alumina with ethylene glycol (EG) and glycerol (GL) precursors are also investegated in detail to assist the interpretation of experimental findings regarding the differences in the hybrid films grown by EG and GL. The DFT calculations show that while the organic precursors can bind to the TMA fragements via formation of Al-O bonds and loss of $CH_4$, it is most favorable for the organic precursors to lie flat and create so-called double reactions through two terminal hydroxyl groups with the surface fragments, where the terminal groups bind to Al. For EG this potentially removes all the active sites and growth will be less favourable. For GL the third hydroxyl group is available and growth can proceed. We also showed that the TMA in the next pulse reacts favourably with this OH from GL. The longer the chain length the harder it is for the organic precursor to stay straight and not create double reactions. This investigation contributes to the understanding of growth process of EG-alucones and GL-alucones at the molecular level and is valuable in supporting experimental data on hybrid film growth.