Modelling Self-Assembly of Phosphonic Acid on Aluminum Oxide Surfaces

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Modeling diffusion controlled processes such as crystal growth remains a challenging task in computational chemistry due to the large time scales. In the Kawska-Zahn approach – a combination of molecular dynamics and Monte-Carlo simulations – the growth is modeled in a

step-by-step process to overcome this problem. [1] In the present work, we present a slightly modified version of this method to investigate the formation of self-assembled monolayers (SAMs) of phosphonic acids on sapphire (0001) surfaces.

As surfactants we considered alkylphosponic acids of various lengths and phosphonic acids containing C60 moieties in different ratios as used by Halik et al. for the formation of self-assembled monolayer field-effect transistors (SAMFETs). [2]

By means of molecular dynamics simulations we demonstrate the gradual ordering of the surfactants during SAM formation, and explore structural/ectronic properties of the bulk Monolayers.

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