

SAMs on α -Al₂O₃(0001): Chemical bonding of linker groups and thermodynamic stability of surface structures

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Al₂O₃ is used in materials science as substrate for self-assembled monolayers (SAM). SAMs play an important role in the construction of novel organic electronic components such as transistors (SAM-FETs) [1,2]. Despite this promising technological use the chemistry at the monolayer-substrate interface is not completely understood. This lack in understanding hinders the purposive design of optimal substrate properties and reaction parameters.

With phase diagrams based on total energy calculations we explain the linkage mechanisms of methyl phosphonic acid and methyl carboxylic acid to α -Al₂O₃(0001) surfaces. We show the dependence of chemical bonding on ambient conditions such as humidity and the dependence of SAM stability on surface structure. We comment on the possibility of α -Al₂O₃(0001) surface reconstruction from its UHV structure to the thermodynamically more stable pseudo gibbsite phase.

[1] M. Halik, A. Hirsch, *Adv Mater* **2011**, 23, 2689-2695.

[2] M. Novak, C. M. Jäger, A. Rumpel, H. Kropp, W. Peukert, T. Clark, M. Halik, *Organic Electronics* **2010**, 11, 1476-1482.