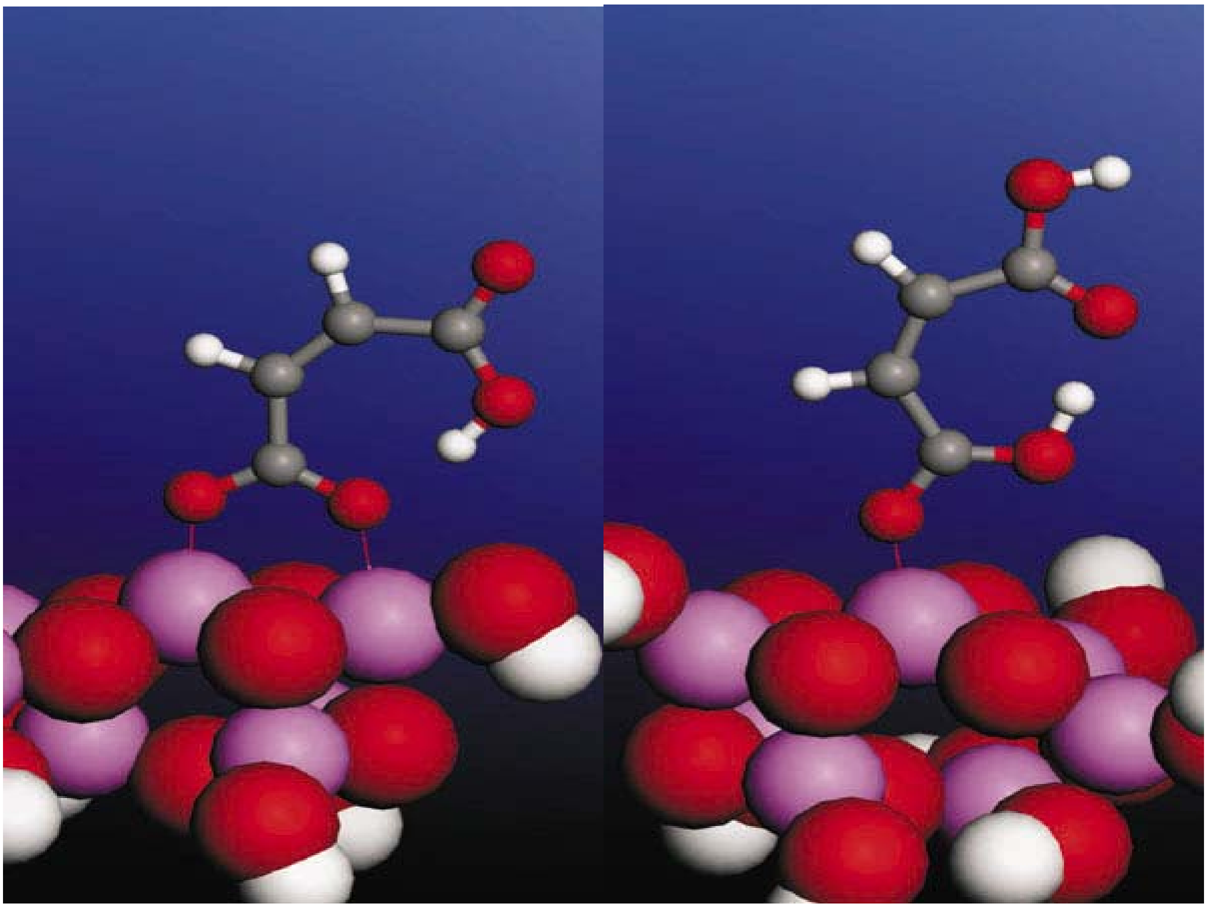
Case SCombined IR/Thermodynamic Study of the Adhesion between Maleic Acid and an Aluminium Surface

Researchers at the Fraunhofer Institute of Applied Materials Research, Bremen, Germany, and The Saarland University, Saarbruecken, Germany, have used Accelrys' DMol 3 in a combined quantum mechanical modeling and IR spectroscopy study of the thermodynamics of the adhesion between maleic acid and an aluminium surface.

This work was awarded the Adhesion Society 2002: Distinguished Paper Award from the The Adhesion Society.



The two types of binding: bidentate (left), monodentate (right)

The principle aims of adhesion science are two-fold: first the mechanical properties of the joint formed must be understood, secondly the long-term durability must be predicted with a certain degree of accuracy. In order to achieve these two aims, studies must focus in on the joint interface and the interphase (the region close to the interface that does not have the properties of the bulk phase).

Commonly used classical models are limited by the fact that in many cases the properties of the joint cannot be accurately predicted. However, molecular modeling, in this case quantum mechanical modeling, offers the opportunity to calculate interface thermodynamic properties which are crucial in understanding the behavior at the interface as well as the interphase.

In a combined quantum mechanical modeling and IR spectroscopy study, Bernhard Schneider of Fraunhofer Institute of Applied Materials Research, and Wulff Possart of the The Saarland University, used Accelrys density functional theory (DFT) program

DMol 3 to investigate the adhesion between a thin film of maleic anhydride and natively oxidized aluminium.

Using DMol 3 , calculated data revealed that the maleic anhydride is hydrolyzed to maleic acid and that the dicarboxylic maleic acid prefers a bridged chelate bond between one acid group and two aluminium atoms on the oxide surface. Further combined investigations revealed that atmospheric humidity changes the chelation to a monodenatate bond between a carbonyl oxygen and on surface aluminium atom.

Dr Bernhard Schneider comments on the value of the computational chemistry techniques used in this work, "We initially wanted to discover which type of bonding occurs between organic thin films and substrate surfaces at the interface. Computation has the advantage that it enables us to expain IR and XPS spectra in much more detail, and understand the adhesive mechanism as well as the related thermodynamics."

"In future we hope to extend the use of computational techniques to calculate the mechanical properties of interfaces and phases, which cannot be obtained by experimental methods."

Reference

1. Thermodynamic Data of Adhasion Phenomena Calculated with Molecular Modeling Methods, Schneider, B.; Possart, W.; Proceedings of the 25th Annual Meeting of the Adhesion Society; 2nd World Congress on Adhesion and Related Phenomena (WCARP-II);February 11-14, Orlando, Fl, (2002), 216.