

Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Understanding Polymer Adhesion: First-principles calculations of the adsorption of organic molecules onto Si surfaces¹ KAREN JOHNSTON, RISTO M. NIEMINEN, Helsinki University of Technology — The adhesion of plastics to ceramics is important for many industrial and technological applications. It is therefore essential to understand the underlying structure and bonding of the polymer and the surface. The aim of this research is to improve plastic adhesion using a multiscale approach. The first step involves the use of density functional calculations to understand the atomic-scale structure and bonding of polymers on surfaces. The plastic of interest is mainly composed of the polymer bisphenol-A-polycarbonate (BPA-PC). The BPA-PC monomer consists of two phenol groups, one propane group and a carbonic acid group. First-principles calculations of the adsorption of these molecules onto the Si(001)-(2×1) dimer surface will be presented. Finally, the incorporation of first-principles data into a coarse-graining method will be discussed.

¹This research is supported by a grant from the Finnish Technology

Karen Johnston
Helsinki University of Technology

Date submitted: 03 Dec 2006

Electronic form version 1.4