

**Effect of Nanoscale Surface Modification on Interfacial Adhesion:
a Theoretical Modelling Study**

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The effects of modification of polyester surfaces on adhesion to carbonaceous solids are investigated using theoretical techniques. Fully atomistic models are constructed of cross-linked polyester and glassy carbon surfaces. Polyester surface modifiers of both the hydrophilic and hydrophobic nature are introduced and simulations are then performed to obtain qualitative and quantitative measures of interfacial strength between the polyester and carbon thin layers [1].

Our studies indicate that Van der Waals forces contribute significantly to the interfacial strength between the thin layers while atomic scale surface roughness is found to significantly reduce adhesion. Interfaces formed from rigid surface models provide general information on structural and chemical effects but such rigid models tend to overestimate the magnitude of these effects. Relaxed interfacial models provide more realistic representations on interactions between the layers. Flexible chain-based modifiers on the surface of the polyester films tend to migrate away from the interface and flatten the surface thereby decreasing the roughness effects on interfacial strength. Both hydrophilic and hydrophobic surface modifications resulted in reduced adhesion at the interface.

[1] Henry D. J., Lukey C. A., Evans E., Yarovsky I., *Mol. Sim.*, *in press*.

Keywords: adhesion, surface modification, molecular modelling