

## Surface Properties of some selected Polymers.

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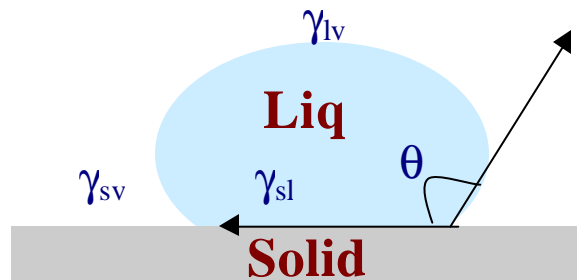
### Abstract:

Wetting and dewetting processes play a very important role in a wide variety of industrial systems, relating to adhesion, compatibility and coatings. The surface free energy of the solid is a characteristic parameter used to determine its wetting properties.

$$\cos \theta = \frac{g_{sv} - g_{sl}}{g_{lv}}$$

**Equation 1** Young's Equation

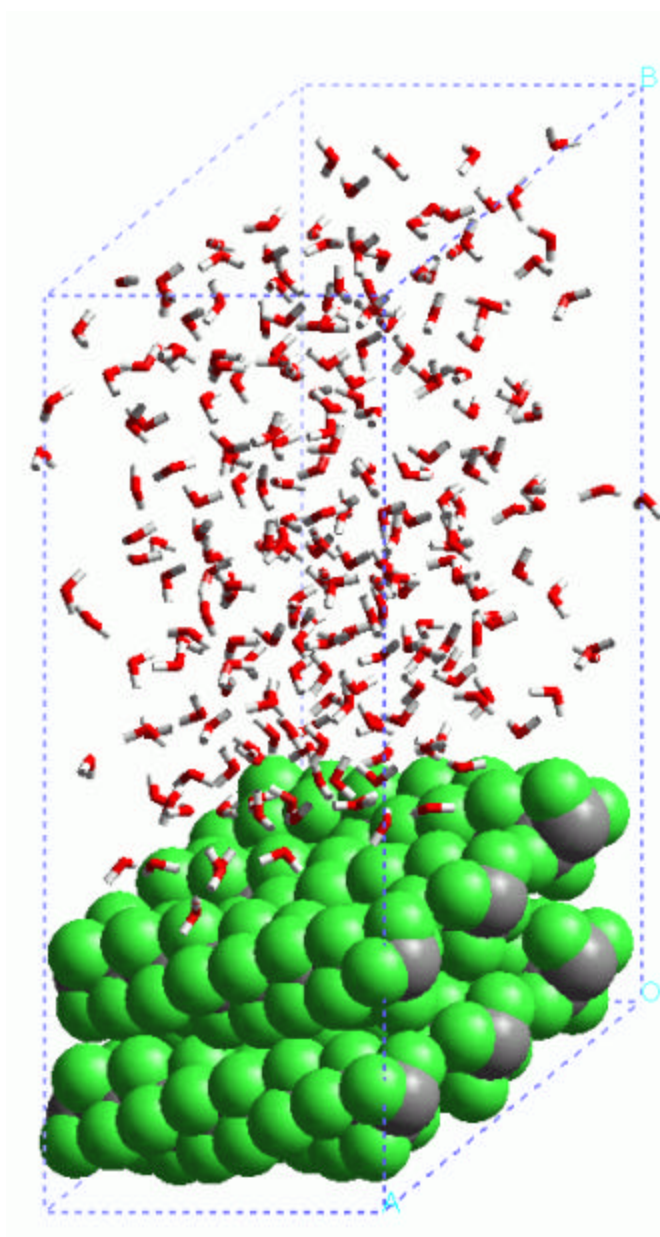
Most wettability tests involve the measurement of contact angles of specific liquids on substrate surfaces. Young's equation relates  $\cos \theta$  to the local balance of forces operating at the three phase line.



**Figure 1** Contact angle of a liquid on a solid surface.

The pathways from measured contact angles to estimated surface free energies is not a fully understood. Zisman introduced the concept of critical surface tension,  $\gamma_c$ , which corresponds to the value of the surface energy of an actual or hypothetical liquid that will just spread on the solid surface giving a non-zero contact angle, however, this is not the free energy of the surface, merely an empirical parameter closely related to the to this quantity.

In order to understand the key properties relating to surface free energy of a solid, molecular dynamic simulations are used to calculate the cohesive energy of the surface of various polymers.



**Figure 2** Water molecules on a PTFE surface.

The interaction energy between a liquid and a solid is also investigated, using both implicit and explicit solvent in an attempt to predict contact angles.