Chapter 1

NEXAFS Spectroscopy

Near Edge X-ray Absorption Fine Structure (NEXAFS) is a method that uses the energy of x-rays to excite electrons into unoccupied orbital levels. Generally, when two electron wavefunctions overlap and hybridise, a bonding orbital and an anti-bonding orbital are formed, which have some energy separation (this was previously covered for polymers in **??**). The bonding orbital is typically occupied (though not always) meaning that transitions can be easily made to the anti-bonding orbital. This forms the basis for many spectroscopic measurements - by aligning incoming X-ray energy to the energy difference between unoccupied orbitals and the anti-bonding levels, information can be gained about the molecular material and it's composition.

1.1 Angle Resolved NEXAFS

Because molecular orbitals have "vector" densities (i.e. ??, ??), polarised X-ray sources have sensitivity and discriminate between various sorts of bonds and orientations.

1.2

Acronyms

NEXAFS The absorption of x-rays by specific core-electrons to unoccupied molecular obitals 1