Critical evaluation of dipolar, acid-base and charge interactions I. Electron displacement within and between molecules, liquids and semiconductors

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Critical evaluation of dipolar, acid-base and charge interactions

I. Electron displacement within and between molecules, liquids and semiconductors

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Abstract

Specific dipolar, acid-base and charge interactions involve electron displacements. For atoms, single bonds and molecules electron displacement is characterized by electronic potential, absolute hardness, electronegativity and electron gap. In addition dissociation, bonding, atomization, formation, ionization, affinity and lattice enthalpies are required to quantify the electron displacement in solids. Semiconductors are characterized by valence and conduction band energies, electron gaps and average Fermi energies which in turn determine Galvani potentials of the bulk, space charge layer and surface states. Electron displacement due to interaction between (probe) molecules, liquids and solids are characterized by parameters such as Hamaker constant, solubility parameter, exchange energy density, surface tension, work of adhesion and immersion. They are determined from permittivity, refractive index, enthalpy of vaporization, molar volume, surface pressure and contact angle. Moreover, acidic and basic probes may form adducts which are adsorbed on target substrates in order to establish an indirect measure of polarity, acidity, basicity or hydrogen bonding. Acidic acceptor numbers (*AN*), basic donor numbers (*DN*), acidic and basic "electrostatic" (*E*) and "covalent" (*C*) parameters determined by enthalpy of adduct formation are considered as general acid-base scales. However, the formal grounds for assignments as dispersive, Lifshitz-van der Waals, polar, acid, base and hydrogen bond interactions are inconsistent. Although correlations are found no of the parameters are mutually fully compatible and moreover the enthalpies of acid-base interaction do not correspond to free energies. In this review the foundations of different acid-base parameters relating to electron displacement within and between (probe) molecules, liquids and (semiconducting) solids are thoroughly investigated and their mutual relationships are evaluated.

Keywords

Electron displacement; acid-base interaction; hydrogen bonding; adduct formation; probe molecules, semiconductors.