Application of Molecular Modelling to Study Nucleation, Impurity Segregation, Solvent Adsorption and Polymorphic Transformation

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Calculating the correct lattice energies is the basis for modelling molecular crystals. The semi-empirical method within the atom-atom formalism has been successfully applied to many organic systems before. Lattice energy of polar crystals like γ-glycine where the electrostatic component plays a vital role could not be evaluated successfully by this method. A combined approach using both semi-empirical and quantum mechanical methods within a periodic formalism has been adopted for successful calculation of lattice energy. Subsequent to this, prediction of crystal shape, additive effect on the host lattice, solvent effect on the surface energies of (hkl) habit faces and energetic stability of polymorphic modifications of the crystal have been modelled. The additive effect on the shape of the host crystal has been studied using semi-empirical method. Segregation coefficient determines the impurity incorporation at the host lattice. Differential binding energy which is proportional to the segregation coefficient can be calculated from the slice and lattice energies. The predicted crystal shapes enable the construction of polyhedral molecular clusters via overlaying the morphological simulation model with the crystal structure. The relationship between the energetic stability and cluster size in polymorphic system, l-glutamic acid has been studied. Further, an attempt has been made via modelling to calculate surface energy values to allow surface dependent (or anisotropic) interfacial tensions to be calculated within the formalism of classical homogeneous nucleation theory.

Keywords: morphology, polyhedral clusters, binding energy