Effective Fragment Potential Method

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Effective fragment potential (EFP) method is based on the decomposition of the system into the active region where an important chemical change takes place (such as bond breaking or electronic excitation) and a number of effective fragments (see Fig. 1.). Active region is described accurately as a quantum system while its interaction with effective fragments is described semi-classically (via one electron terms in the Hamiltonian) using a polarized force filed. One of the strengths of the effective fragment potential is that the polarized force field, which is responsible for intermolecular interaction is also obtained from the ab initio computation on the individual effective fragments and its quality could be improved systematically. Typical molecular systems, which could be modeled with effective fragment potential method are: (1) molecules in solvent (for instance, an amino-acid in cell cytoplasm) and (2) molecular clusters (for example, water clusters).

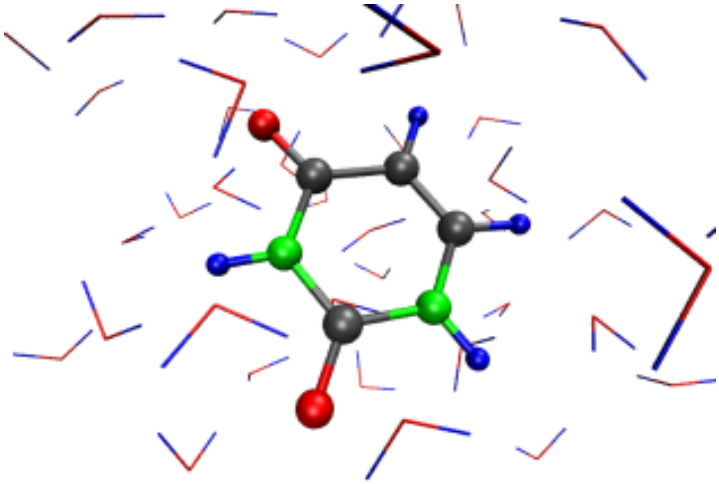

Fig 1: Uracil molecule in aqueous solution. Active region (uracil) is shown with *balls and sticks* model. Effective fragments (water) are shown with *lines* model.