Effective Fragment Potentials for non-rigid fragments

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The Effective Fragment Potential (EFP) method is a computationally accurate and efficient way to describe intermolecular interactions in condensed-phase systems. EFP is a model potential that decomposes non-covalent interaction energy into electrostatic, polarization, dispersion, and exchange-repulsion components, all of which are directly derived from the first principles. Recently, we extended the EFP method to model non-covalent interactions in macromolecules and polymers such as proteins and DNA. However current EFP implementation is not suitable for large scale simulations due to its inherent limitation of representing effective fragments as rigid structures. Thus, the process of obtaining EFP parameters in a system with flexible degrees of freedom entails multiple sets of *ab initio* calculations and requires intensive computational resources. To circumvent this issue, we formulate a computational approach that can efficiently utilize EFP for flexible molecules, so called Flexible EFP. We demonstrate computational efficiency and accuracy of Flexible EFP on extensive examples of amino acid interaction energies and electronic properties of Flavin chromophore of the cytochrome protein.