

MS36-2-1 HirshFrag: a new software tool for automatic molecular fragmentation
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Abstract

Hirshfeld Atom Refinement (HAR) [1, 2] is becoming more and more important in the refinement of single crystal X-ray data. However, the use of quantum chemical calculations is the main bottleneck in HAR. It is well-known that the computational chemistry methods are still very limited in applicability to many systems of interests such as proteins and polymers. One of the most effective strategies to make such computations feasible is to use the fragmentation methods [3-6]. By the fragmentation method, we mean the partition of a large system into effective overlapping or non-overlapping subsystems (fragments), performing quantum chemical calculations for each fragment, and combining the fragments together to compute properties of the whole system. We have developed a new code called HirshFrag, which is intended for the automatic molecular fragmentation. The code employs several different methods of molecular fragmentation including the Systematic Molecular Fragmentation [4, 5] with some improvements, and an approach developed in our group [6]. The current version of HirshFrag is able to interact with the discamb2tsc program from the DiSCaMB software package [7].

In this presentation, we will discuss how different fragmentation approaches, available from HirshFrag, influence on HAR. In addition, we will discuss the speed up that can be achieved thanks to the fragmentation.

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