Towards Accurate Calculations on Large Molecular Systems

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Abstract

In order to performa accurate electronic structure calculations on large molecular species and processes, such as solvated ions, heterogeneous catalysis, and solvent effects on chemical reactions and spectroscopy, one must develop novel approaches. One such approach is collectively called fragmentation methods. A suite of fragmentation methods, the effective fragment potential, fragment molecular orbital, and effective fragment molecular orbital methods will be discussed, with examples.