Molecular Tailoring Approach : An Art of the Possible for *ab initio* Treatment of Large Molecules and Clusters

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The formidability of implementing large molecular calculations using these methods will be discussed. Divide-and-conquer (DC) type methods are being actively developed [1] in order to break this bottleneck of high scaling order of *ab initio* calculations of large molecules. Molecular Tailoring Approach (MTA) is one of such early attempts, which scissors the parent molecular system into subsystems (fragments) [2], the properties which are stitched back in order to estimate those for the parent system. Incorporation of the inclusion-exclusion principle into MTA allows accurate estimation of molecular properties, electronic energy, energy-gradients and Hessian.[3] The basic methodology of MTA will be summarized, along with applications to a variety of test systems. It will also highlight the versatility of this method with respect to the level of theory and basis-set. Apart from the earlier benchmarks, some newer results on geometry optimization and molecular properties of a variety of molecular clusters [5], polyaromatic hydrocarbons [6], water clusters and a protein with charged centers will be discussed. This will be followed by an account of the recently developed molecular cluster building and topography mapping algorithms, along with some examples.

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