Treating Large Molecules and Clusters by ab initio methods: an Art of the Possible

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Abstract

Molecular tailoring approach (MTA), a fragmentation-based method developed in my laboratory will be discussed. In the first part of the talk, I will show applications of the method for calculating molecular electron density (MED) and molecular electrostatic potential (MESP) of large molecules. The second part of the talk will discuss geometry optimization and calculations of IR and vibrational Raman spectra with MTA. Several illustrative examples will be presented.

N. Sahu & S.R. Gadre, Molecular tailoring approach: a route for *ab initio* treatment of large clusters, Acc. Chem. Res. 74, **2014**, 2739