New developments and applications of the generalized energy-based fragmentation approach

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In this talk, I will present our recent developments and applications of the generalized energy-based fragmentation (GEBF) approach, which provide a fast and reliable theoretical tool for approximate *ab initio* calculations of very large molecules.[1-3] The essence of this method is to divide a large molecule into many fragments and obtain the approximate ground-state energy or properties of this molecule from the corresponding quantities of various "electronically embedded" subsystems. Very recently, an automatic algorithm for partitioning a large system has been accomplished,[4] which allows the applications of the GEBF approach to be available by non-expert users. With the newly implemented GEBF approach, one can compute energies, optimized structures, vibrational spectra, and some molecular properties of very large systems at various *ab initio* levels on ordinary PC workstations. The GEBF approach has been applied to investigate several interesting chemical problems in large systems, such as the driving forces of molecular self-assembling processes,[5] low-lying structures and stabilities of large water clusters,[6] and the structures, energies and enthalpies of helical structures for capped polyalanines with up to 40 residues.[7]

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