Prospects of Protein Calculations by the Density Functional Theory

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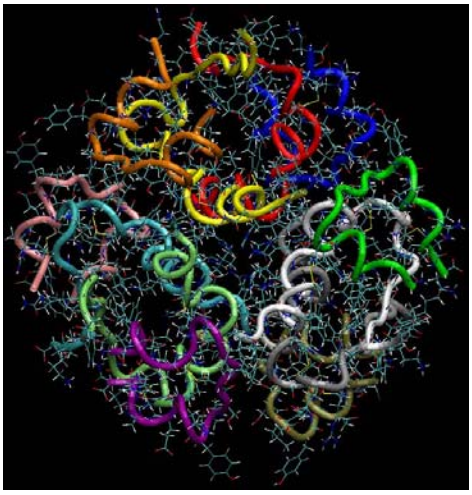
We have developed ProteinDF program with the Density Functional Theory to calculate the electronic structure of proteins[1-3]. By using this program, an all-electron calculation on the non-symmetric insulin hexamer(see figure) was successfully carried out[4,5] with a precise initial guess of the combined quasi-canonical localized orbitals[6]. The numbers of residues, atoms, and orbitals were 306, 4728, and 26790, respectively. To our knowledge, insulin hexamer is the largest system calculated using the full-scale canonical density functional molecular orbital method.

On the base of such experience, the future of protein calculations by the density functional theory will be discussed.



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