Applications of Large-Scale Electronic Structure Calculations in Biology

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Recent progress in linear-scaling density functional theory (DFT) software allows electronic structure calculations of systems comprising many thousands of atoms to be performed on a routine basis [1], allowing access to typical length-scales in many biomolecules. In this talk, I will give examples of some of the areas in the biological sciences where DFT can play a role - from the energetics of chemical reactions in enzymes [2] and binding of small molecules by metalloproteins [3,4], to the parameterisation of model Hamiltonians to describe energy transfer in photosynthetic light-harvesting complexes [5] and drug development in medicinal chemistry [6].

[1] www.onetep.org/


