Large-scale DFT calculations on biological systems with the CONQUEST code

T. Miyazaki¹, T. Otsuka¹, M. Todorovic¹, T. Ohno¹, D. R. Bowler², and M. J. Gillan²

¹Computational Materials Science Center, National Institute for Materials Science, Tsukuba, Ibaraki, Japan
²Department of Physics and Astronomy, University College London, London, United Kingdom

We report our recent study on biological systems using a linear-scaling (or O(N)) DFT code CONQUEST. The code is efficient on massively parallel computers and has an ability to treat systems containing many thousands of atoms. CONQUEST minimizes DFT total energy with respect to the Kohn-Sham density matrix and it can be run at different levels of precision ranging from ab initio tight binding to full DFT with planewave accuracy. With these abilities, we have recently succeeded in atomic relaxation of the nano-structured Ge 3D islands on Si(001), which contains more than 20,000 atoms.

Here, we present our recent studies on 1) hydrated DNA and 2) membrane protein systems. In both studies, pseudo atomic orbitals (PAOs) are used as basis sets. We first investigate the accuracy of the basis sets with DZP quality and have found that they give satisfactory results. It has been also confirmed that GGA-PBE is fairly accurate to express the hydrogen bonds in DNA systems.

For 1), we have performed order-N DFT calculations on a DNA decamer system surrounded by a large number of water molecules (upper figure). The system consists of 3439 atoms; 634 atoms for a DNA decamer, 9 Mg counter ions and 932 water molecules. We have found that the DFT calculations are robust and that the density
matrix minimization method used in the O(N) calculations is fairly accurate. The
dependence of the total energy on the cutoff radius of the (auxiliary) density matrix is
shown in the lower figure and we can see that the energy converges very rapidly. We
have also compared the calculated forces by CONQUEST with those by AMBER.
Detailed analysis will be given in the talk.

For 2), we are currently working on isolated gramicidin-A protein. Gramicidin-A is a
small but highly selective ion channel, whose inner pore conducts only monovalent
cations. We explore the ground-state geometry of this system by performing structure
relaxations from two experimental atomic configurations, which have different helix
properties and peptide residue orientation. Furthermore, we study the effect of peptide
side-chains on the geometry and electronic properties of this system by replacing all
side-chains with methyl groups (thus generating an artificial alanine channel). Although
the conventional diagonalisation method is mainly used in the study of the isolated
molecule, we demonstrate the accuracy of the order-N method necessary for our future
modelling work on the ion channel embedded in a solvated phospholipid membrane.

We acknowledge A. S. Torralba (NIMS) and V. Brazdova (UCL) for the useful
discussion and their contributions in the development of the code. The present work is
partly supported by Grant-in-Aid for Scientific Research, KAKENHI (17064017 and
20540401).

177, 14 (2007)
(2007).