Developments and applications of a linear-scaling DFT code CONQUEST

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We report our recent progress in developments and applications of our linear-scaling DFT code CONQUEST. The code is efficient on massively parallel computers and has an ability to treat the systems containing more than ten thousands of atoms. The code is based on the strategy of minimizing the total energy with respect to the Kohn-Sham density matrix, and the practical techniques for implementing this strategy will be briefly summarized. The code can be run at different levels of precision, ranging from empirical tight-binding, through ab initio tight-binding, to full plane-wave precision, and the way in which this is achieved will be outlined.

As one of the research example by CONQUEST, we show our theoretical study on the nanostructured Ge 3D islands on Si(001). We demonstrate that it is now possible to perform DFT calculations on such large and scientifically important systems. We have succeeded in employing DFT structure optimization on the systems containing more than 20,000 atoms. We are also using the code for the study on biological systems, and in preparation for large-scale calculations on DNA systems, we have recently calculated single DNA bases and on DNA base pairs and compared the results with those obtained by other codes. The results of these test calculations will be given with our future targets.

We have recently released the beta version of the code. We plan to release the code under a GNU General Public Licence soon. The present work has been done in collaboration with M. Todorovic (NIMS), A. S. Torralba (UCL) and V. Brazdova (UCL), and is partly supported by the Grant-in-Aid for Scientific Research on Priority Areas from MEXT.