The K Supercomputer and Recent Advances in LC-DFT

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Twice a year, the world's supercomputers are ranked according to their level of performance in a listing called the TOP500. On June 20, 2011, the K computer jointly developed by RIKEN and Fujitsu was pronounced the fastest computer in the world in the TOP500 listing announced at the 2011 International Supercomputing Conference in Hamburg. The K computer came out way ahead of its competitors with a LINPACK benchmark performance of 8.162 petaflops. The K computer's achievement was wonderful news following as it did the devastation of the March 11 Great East Japan Earthquake, and reinforces Japan's strengths in science, technology and manufacturing. It is my fervent hope that the international recognition given to the K computer will help to prime Japan's recovery from the disaster. It should be noted, however, the real test of the K computer will be the results that are achieved through its use. With the emergence of petascale computing platforms we are entering a new era of modeling. Petascale computing will enable us to simulate physical processes on a scale never seen before, and approach convergence for dynamical processes never thought possible. The K computer will open up a new frontier in computational chemistry.

DFT has emerged as a powerful computational tool for the chemical systems. It is simple and conceptual. KS-DFT calculation takes about the same amount of time as a HF calculation, yet unlike HF, we get a correlated result from KS-DFT. Many of the problems of KS-DFT have mostly been a consequence of not having accurate functionals and potentials. Recently there has been considerable interest in the long-range correction (LC) DFT. In the LC scheme the exchange functional is partitioned with respect to the inter-electronic separation into long-range and short-range parts using a standard error function. The LC solves many of the problems of the conventional KS-DFT. Recently it was demonstrated that the LC satisfies Koopmans'theorem, which implies that the eigenvalues and eigenvectors connected to the Kohn-Sham equation have a strict physical meaning. Different from Hartree-Fock Koopmans ionization energy, DFT Koopmans ionization energy to some extent takes into account the relaxation and correlation effects. Recent advances in LC-DFT will be discussed.