

Project Summary

We propose the purchase of a high performance parallel computer to be located in the Department of Chemistry at Michigan State University. The proposed computer is an important step in the continuing integration of computers and computing into the research, teaching and outreach activities of the department. It will greatly enhance the ability of faculty and students in the MSU chemistry department to continue the development and effective use of modern electronic structure techniques in their research. Many applications that are of interest to us involve large biologically significant molecules, solids, or small molecules that must be treated at a very high level of theory. All of these applications and the ongoing technique development activities will benefit from the proposed 16 CPU, shared memory computer.