Department of Energy
Office of Science
Washington, DC 20585

Office of the Director

October 17, 2003

Professor John Hemminger
Department of Chemistry
University of California, Irvine
Irvine, CA 92697

Dear Professor Hemminger:

Thank you very much for agreeing to chair the Basic Energy Sciences Advisory Committee (BESAC). I very much appreciate you taking on this important function for the Office of Science. This year, I would like BESAC to take on two charges:

1. The August 10, 1999, charge to BESAC instituted Committees of Visitors (COV) to assess the program management of major elements of the Basic Energy Sciences (BES) program every three to four years. The first two COV reviews–of the chemical sciences research activities in January 2002 and the materials sciences and engineering research activities in March 2003–resulted in many improvements to the peer review process. These reviews were of great benefit to the BES program managers and to me. I know that you served as a member of the first COV review and the Chair of the second, and I want to thank you for your help in establishing COVs in the Office of Science. I would now ask BESAC to conduct a COV review of the activities within the new Scientific User Facilities Division. A report to BESAC should be planned for the summer or fall 2004 BESAC meeting.

2. Next, I would like BESAC to empanel a subcommittee to consider theory, high-end computing, work-station/cluster computing, and algorithm development as they pertain to the research activities of the BES programs. Although there have been several such studies in the recent past, none were specific to the BES research communities and none sought to comprehensively look at all of these elements simultaneously. The subpanel should have at least one member of the Advanced Scientific Computing Advisory Committee to provide liaison with that group. You should work with the subcommittee chair to refine a charge; however, at a minimum, I would like the study to address the following:

(a) Identify and assess the major opportunities to advance the research supported by the Basic Energy Sciences program through high-end computing (HEC) and through conventional (workstation and cluster) computing. Summarize recent past and projected future scientific impacts of each.

(b) Identify research areas supported by the Basic Energy Sciences program that are now using HEC, are ready to use HEC, or that might benefit from HEC in the near future. Assess the challenges and needs for the use of HEC, e.g., the development of theory, mathematical algorithms, system software, and hardware architectures; the availability of and access to HEC machines and the customization of HEC machines; and the funding requirements.

Please provide a bibliography of recent, relevant studies that you encounter in this study.

Sincerely,

Raymond L. Orbach
Director
Office of Science