Department of Energy
Office of Science
Washington, DC 20585

Office of the Director

January 25, 2005

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

Dear Professor Hemminger:

Thank you very much for your continuing service to the Office of Science (SC) and the scientific communities that it serves as the Chair of the Basic Energy Sciences Advisory Committee (BESAC). I realize that the last several months have been difficult as we have worked to transition the advisory committees from representational membership to expert membership. Let me assure you that we are working to make this change as smooth as possible. I want to thank you for your help and understanding during this transition period.

I am writing to charge BESAC with an interesting project, somewhat unlike those that you have addressed in the recent past. Over the past century, multiple scientific disciplines – all dependent on understanding and controlling assemblages of atoms – have matured nearly simultaneously. Atomic and molecular physics, condensed matter physics, materials physics, chemistry, molecular biology, geoscience, and environmental science are but a few. All of these are represented in the BES portfolio.

Much of the research in these fields has been devoted to solving difficult problems for idealized, simple systems. Profound insight into both the nonliving and living worlds has resulted. However, in recent years, it has become clear that there are a multitude of fascinating and useful properties that arise because of complexity and cooperative behavior among parts of a system. The effects are seen in systems as diverse as high-temperature superconductors; soft materials such as surfactants, liquid crystals, microemulsions, colloids, and macromolecules; self assembled systems; and, of course, living systems.

Each of the disciplines supported by BES has come to require a detailed quantitative understanding of atomic-level behavior of materials. Further, each has struggled with questions that appear to be beyond the scope of current theories and of present experimental and computational tools. These questions often transcend individual areas of study leading to common themes and unifying concepts.

The number of worthy questions, and the theories and experimental approaches used to address them across the BES portfolio, have become so large that it is often difficult to grasp the "big picture". The time has come to develop a new way of describing these challenges, anchored on a finite set of big questions, illuminating the full scope for BES science.

I am asking BESAC to sponsor a workshop entitled **"How atomic assemblies govern the world we live in: Key scientific questions for the Basic Energy Sciences"**, perhaps in conjunction with a future BESAC meeting, with the following goals:

1. **Identify and articulate for the broader scientific community the most important scientific questions and science-driven technical challenges facing the disciplines supported by BES.** The challenges should be limited in number to perhaps one dozen and should be described in a manner that is independent of current disciplinary labels and of terms such as "multidisciplinary" or "interdisciplinary." These challenges should arise from major gaps in our understanding, future discovery potential, and excitement of the quest.

2. **Describe the importance of these challenges to advances in disciplinary science, to technology development, and to energy and other societal needs.**

3. **Describe what might be needed to address these challenges, including the development of theories, instruments, facilities, and computational capabilities and education and workforce development.**

4. **Connect the challenges with disciplines outside of those supported by BES, as appropriate.**

5. **Use as resource material previous discussions at BESAC and relevant studies by BESAC, other SC Advisory Committees, the NRC, and other bodies.**

6. **Suggest follow-on activities, as appropriate.**

This activity is intended to convey the essence and potential of BES science in a set of compelling questions. It is not intended to produce an inventory of research being done or planned. It is meant to stimulate discussion and, as appropriate, to prompt further studies by the SC Advisory Committees and other bodies. I know that you already have had several discussions on this topic during recent BESAC meetings. The list of questions that you discussed at your last meeting might be considered a starting point; however, do not feel bound by this list.

The output of this workshop should be a brief report with an Executive Summary suitable for a general audience. The report should be available in the fall of 2005.

Sincerely,

Raymond L. Orbach

Raymond L. Orbach
Director
Office of Science