NSF-sponsored workshop on Materials by Design

March 17th to 19th, 2011
Loma Pelona Center, University of California, Santa Barbara

http://www.mbd.mrl.ucsb.edu/

Some questions to be addressed:

1. How can the community at large, and the NSF specifically, respond to weakening leadership in the synthesis/growth of advanced materials as discussed in the NRC report: Materials that push the boundaries of condensed matter and materials physics. Has the loss of some traditional strength been associated with the development of new ones? What can we do to reestablish those traditional strengths that still add value to the community? The NRC report carefully underscores the relationship between crystal growth and development of new technologies. In this regard all participants should underscore what we bring to the table in terms of stating the value of our science.

2. What kind of infrastructure (compatible with the NRC report recommendations) is needed for MbD, and how can it be used to further collaboration, competitiveness, and education.

3. Specifically for MbD, how can computation and theory interact more effectively, and how could the recommended Discovery and Growth of Crystalline Materials (DGCM) network proposed in the NRC report act to facilitate such an interaction.

4. The NRC report specifically draws attention to activities such as MBE growth, crystal growth in extreme environments, and crystal growth for specialized applications as not fully supported, especially in an academic environment. How can funding programs support such activities through academic programs, and what would be the relationship with federally funded labs and facilities.

7. When does MbD diverge from DGCM? Obvious places are soft matter, amorphous materials (glass), and nanoscience. Question: What is the U.S. research competitiveness in these areas and how is it balanced by present funding and by future economic opportunities?

8. Many of the processes for the assembly of soft materials mimic those of traditional crystal growth. Is there sufficient communication between these research communities and should programs be developed to bridge the gaps between these disciplines?

9. What is the status of theory in organic electronics?

10. Databases of crystal structures – the ICSD, the Cambridge Database, the Pauling File, the PDB, *etc*. exist, as do databases on structural materials (Ashby maps) or NIST ceramics phase diagrams. What about databases for functional material properties? Is it a useful exercise to compile materials properties (such as is done by Landolt-Börnstein): room and low-temperature mobilities, resistivities, and Seebeck coefficients, superconducting T_C's, band or HOMO-LUMO gaps *etc*. for hard and soft materials, and make them accessible *via* a database search. Would this be a job for the DGCM Network administration?