The next two days we can only touch upon the highlights of the enormous progress over the last year at the MSC. This progress is due both to the high quality of the postdoctoral staff and the students (including undergraduates) at Caltech and to the very fruitful interactions with our industrial collaborators and our universities collaborations. Some of the highlights follow.

Advances in theory and methods are making it practical to consider fully first principles (de novo) predictions of a broader range of important systems and processes in the Chemical, Biological, and Materials Sciences. Critical to this process is connecting the quite different paradigms used in QM, FF based MD, meso scale simulations, and the finite element approaches used in continuum descriptions of macroscale systems. With funding from DARPA we have built the The Computational Materials Design Facility (CMDF) to facilitate combining the results of incompatable codes on the same problem (thus describing a propagating crack in Si crystal using QM at the crack tip, ReaxFF near the propagating crack, and more ordinary FF far from the crack). This is now the foundation of the PROM (predicting real optimized materials) DARPA project. This involves teams from JPL, USC, and elsewhere working with us to predict figures of merit for thermoelectrics, ferroelectric switches, nonlinear optical systems, and propellents.

Highlights of this meeting include advances in
- the methodology for predicting protein structures of membrane-bound proteins (GPCRs) and ligand binding. This is the basis for new collaborations with Pharma (Aventis-Sonafi and Berlex with others under discussion).
- Reactive Force Fields (ReaxFF) to describe catalytic reactions and phase transitions. This is the basis for a new collaboration with Nissan Corp.
- Fuel Cell Catalysts and Membranes:
- Nanoelectronics: Prediction of current/voltage in nanoelectronic devices. This is the basis of a new collaboration with Intel.
- New materials for molecular electronics
- Homogeneous catalysts for selective reactions
- Advances in Power, Energy, Environmental Research (PEER)