

Final report for grant: DE-SC0004028 (UCB Fund# 30168):

This grant was \$12500 for partial support of an international conference, Molecular Quantum Mechanics 2010, which was held on the campus of the University of California, Berkeley, from 24 to 29 May 2010. The conference involved more than 250 participants. The conference schedule ran from as early as 8:00 AM to as late as 10:30 PM at night, in order to accommodate six historical lectures, 16 plenary lectures, 42 invited talks and two very strong poster sessions containing 143 contributed posters.

Since 1989, the Molecular Quantum Mechanics (MQM) series of international conferences has showcased the frontiers of research in quantum chemistry with a strong focus on basic theory and algorithms, as well as highlights of topical applications. Both were strongly in evidence at MQM 2010. At the same time as embracing the future, the MQM conferences also honour the lifetime contributions of some of the most prominent scientists in the field of theoretical and computational quantum chemistry. MQM 2010 recognised the work of Prof. Henry F. 'Fritz' Schaefer of the Center for Computational Chemistry at the University of Georgia, who was previously on the faculty at Berkeley.

The travel of invited speakers was partially covered by sponsorships from Dell Computer, Hewlett-Packard, Journal of Chemical Theory and Computation, Virginia Tech College of Science, Molecular Physics, Q-Chem Inc and the American Institute of Physics.

By contrast, the conference grant from the Department of Energy was used to provide fellowships and scholarships to enable graduate students and postdoctoral fellows to attend the meeting, and thereby broaden the participation of young scientists at a meeting where in the past most of the attendees have been more senior faculty researchers. We believe that we were very successful in this regard: 118 students and postdocs attended out of the total of 256 participants.

In detail, the DOE sponsorship money was partially used for dormitory scholarships that covered the cost of shared accommodation for students and postdocs at Berkeley dormitories. This covered the \$200-\$305 cost of a shared room for the 5-day duration of the conference. The only condition of these scholarships was that the awardee must present a poster at the meeting. Approximately \$7565 was spent for these dormitory scholarships. The remaining expenditures of \$4800 was used for 12 merit scholarships which were awarded to students whose poster presentations were judged the best at the conference. This amount covered a significant part of their travel and registration fees.