iQUEST Annual Report, 2004-2005

Director's Statement

It has been a year of change and transformation at iQUEST. Beginning July 1, 2004, iQUEST began managing extramural contracts and grants for the Department of Chemistry and Biochemistry (DCB) in addition to those of its current principal investigators. In order to handle the huge increase in workload, two additional administrative staff were hired, bringing the total to five. In the end of August, iQUEST moved from a trailer in front of the library to newly renovated offices on the third floor of Broida Hall. Finally, to reflect its new identity, and after consultation with the Advisory Committee, the Office of Research, the Academic Senate, and the chairs and members of many academic departments, iQUEST decided to change its name to the institute for Quantum and Complex Dynamics (iQCD), effective July 1, 2005. Thus, this will be the final annual report from iQUEST. Next year's will be the first from iQCD.

Much of the story of the last two years is evident from the following numbers:

	2003-2004	2004-2005
Number of proposals submitted	33	122
Total value of submitted proposals	$15.8M	$45.4M
Number of awards received	15	58
Value of awards received	$3.2M	$8.4M
Total number of awards administered	32	93
Total value of awards administered	$15.1M	$40.3M

The growth from last year is entirely associated with the addition of proposals and awards from the DCB to iQUEST's portfolio.

The numbers of course don't tell the whole story. Each and every proposal is different, is associated with a tremendous amount of work and co-operation between the PI and staff, and has a deadline (always met, but generally not with much time to spare despite the staff's best efforts to train the PIs). When the good news comes that a proposal has been awarded, iQUEST has been proud of its careful stewardship of the funds, and the people and purchases that the award supports.

The transition of existing DCB awards to iQUEST's accounting system was a Herculean task which required months, long hours, and painstaking attention to detail. A milestone of this transition occurred in February 2005, when updated easy-to-read monthly statements for each award were made available online to every PI. PIs no longer need to wait for monthly statements in print, but can check their accounts at any time from their desktop computer.

Ultimately, of course, the goal of an Organized Research Unit (ORU) is to facilitate world-class research. It is impossible to do justice in this brief report to the vast amount of research carried out using funds administered by iQUEST. Here is just one research highlight, a paper entitled "Conversion of large-amplitude vibration to electron excitation at a metal surface" [Jason D. White, Jun Chen, Daniel Matsiev, Daniel J. Auerbach, and Alec M. Wodtke, Nature **433**, 503 (2005)]. In this paper, diatomic molecules with large-amplitude vibrations were fired at a metal surface in ultra-high vacuum. A diatomic molecule consists of two atoms, and can be thought of as a dumbbell in which the weights are connected by a spring. Upon striking the surface, these vibrating molecules directly transferred the energy associated with their vibration to electrons in the metal, and caused electrons to be ejected from the surface. Atoms and their nuclei are much heavier than electrons, and hence move much more slowly. It has been commonly assumed that light and nimble electrons simply "follow" the motion of relatively sluggish vibrating atoms in molecules. This assumption was translated into a very useful theoretical approximation by Born and Oppenheimer (before Oppenheimer became head of the Manhattan project). The result of this paper shows that the widely-used Born-Oppenheimer approximation does not work when vibrating molecules strike a metal surface. New theory will need to be developed to explain this experimental result. Experimental scientists love nothing more than to send their theoretical colleagues back to the drawing board.