Final Scientific Report on ``Theories of Strong Electron Correlations in Molecules and Solids'' - DE-FG02-97ER45640

PI: Daniel L Cox, Department of Physics UC Davis

Summary

This was the final award period for a grant the PI first received as an assistant professor at Ohio State in 1987, and contributed significantly to his work on high temperature superconductivity, exotic Kondo effects in metals, electron transfer and transport in DNA, and strong correlation effects in organometallic/biomimetic molecules. Over the 21 years of this award and its antecedents, support has been given to 15 postdoctoral researchers, and 13 PhD students. Of the PhD students five have secured positions in research universities, three in colleges or masters level universities, three in technology/science related industry positions, and one in financial modeling. Of the postdoctoral researchers, eight have secured positions at research universities, one at an undergraduate institution, two in industrial research, one at a national lab, and three in financial modeling. Over the years this grant has led to 104 publications in the form of journal articles, theses/dissertations, or books. Among these are the highly cited publications:

(DE/ER/45640-92) "The Quest for High Conductance DNA", R.G. Endres, D.L. Cox, R.R.P. Singh, Rev. Mod. Phys. **76** 195 (2004) – 423 ISI Citations (This paper has helped set the stage for all subsequent work on electron transfer/transport in DNA)

(DE/ER/45640-77) "*Exotic Kondo Effects in Metals*" D.L. Cox and A. Zawadowski, Adv. Physics. **47** 599 (1997), - 346 ISI Citations (This is the go to reference still, for exotic quantum impurity physics in metals)

"EVIDENCE FOR NON-FERMI-LIQUID BEHAVIOR IN THE KONDO ALLOY Y1-XUXPD3" C.L. Seaman, M.B. Maple.... D.L. Cox, Phys. Rev. Lett. **67** 2882 (1991). 305 ISI Citations (This paper helped create the field of non-Fermi liquid metals in heavy fermion systems)

In the final period of the grant the PI led work on correlated hybridization in metals, molecules, and molecular transistors, work on the electron transfer of MutY to DNA, work on electron transport in DNA between gold electrodes. Hoped for work on zintl compounds, dependence of DNA results on water potentials, and the Yb Kondo valence change system did not reach fruition in the no cost extension year of the award as junior personnel took available job opportunities.

Publications 2005-2009

DE/ER/45640-100 - [Correlated Hybridization in Transition-Metal Complexes](#), A. Huebsch, J.C. Lin, J. Pan, and D.L. Cox, Phys. Rev. Lett. **96**, 249901 (2006).

DE/ER/45640-101 J.C. Lin, F.B. Anders, D.L. Cox, **Influence of correlated hybridization on the conductance of molecular transistors**, *Phys. Rev. B* **76**, 115401 (2007).

DE/ER/45640-102 ``Sequence Dependent Electron Transport in Wet DNA: Ab initio and Molecular Dynamics Studies'' has been published in Physical Review Letters (Physical Review Letters **101**, 176805 (2008)) and also in the Virtual Journal of Biological Physics Research and Virtual Journal of Nanoscience and Technology.

DE/ER/45640-103 *Theoretical study of DNA damage recognition via electron transfer from the [4Fe-4S] complex of MutY* has been published in Biophysical Journal (Biophys. J. **95**, 3259-3268 [2008]).

DE/ER/45640-104 J.C. Lin, *Quantum Mechanical Studies of Transition Metal Complexes in Organometallic Molecules: From Metalloproteins to Molecular Transistors* (PhD dissertation, UC Davis Department of Physics, 2008)

Personnel who received partial support during 2005-2009

Dr. Kay Kunes is a staff scientist with Raytheon Corporation in Tucson (since Aug. 2009).

Dr. Cynthia Trevisan is a lecturer at California Maritime Academy (since summer 2008).

Dr. David Mobley is now a professor of pharmaceutical chemistry at the University of California, Irvine [Sept. 2012] (**DE/ER/45640-94,95**)

Dr. Frithjof Anders is now a full professor of physics at the University of Dortmund [Nov. 2008] (**DE/ER/45640-88, DE/ER/45640-101, DE/ER/45640-82, DE/ER/45640-67, DE/ER/45640-69, DE/ER/45640-66, DE/ER/45640-61**)

Dr. Montego LaBute is a staff scientist at Lawrence Livermore National Labs [since 2011] (**DE/ER/45640-91, DE/ER/45640-96, DE/ER/45640-89**)

Dr. Robert Endres is a lecturer in computational biology at Imperial College in London [Sept. 2007] (**DE/ER/45640-98, DE/ER/45640-91, DE/ER/45640-96, DE/ER/45640-90, DE/ER/45640-92, DE/ER/45640-93, DE/ER/45640-75**)

Dr. Jong-chin Lin is a postdoctoral researcher with Dev Thirumalai at U of Maryland.

Dr. Jianping Pan is a financial modeler with Credit Suisse [June 2008] (**DE/ER/45640-100**).

Dr. Arnd Huebsch is a consultant with D-Fine in Germany [Sept. 2007] (**DE/ER/45640-98, DE/ER/45640-100**)

Invited presentations associated with the award during 2005-2009

Correlated hybridization in transition metal complexes, A. Huebsch, Leibniz Institute, Dresden, March 2006

Correlated hybridization in transition metal complexes, A. Huebsch, Max Planck Institute for Complex Systems, Dresden, Nov. 2005

Electronic properties of DNA in solution and in vivo, D.L. Cox, Quantum coherence and biomolecular dynamics, International ICAM workshop, Queensland Australia, April. 2007.

Strong correlation effects in Transition Metal Complexes, D.L. Cox, Quantum coherence and biomolecular dynamics, International ICAM workshop, Queensland Australia, April. 2007.

Electronic properties of DNA: theoretical studies in solution and biological environments. D.L. Cox, American Chemical Society Fall Meeting, August. 2007, Boston MA