Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

How does thermal motion of atoms influence the rates of bridge-mediated electron transfer reactions? 2. Examination for Frank-Condon approximation. TUSTOMU KAWATSU, Duke University, SPYROS SKOURTIS, University of Cyprus, ILYA BALABIN, DAVID BERATAN, Duke University — Bridge-mediated long-range electron transfer (ET) is ubiquitous in biological systems. The ET reaction rate is generally calculated using Born-Oppenheimer and Franck-Condon approximations. We focus on the validity of the Frank-Condon approximation and estimated how well it describes protein ET for Ruthenium-modified azurins. We compare the auto-correlation function decay time for the electronic coupling with the decay time of the Franck-Condon factor (computed by D. M. Lockwood, Y-K. Cheng and P. J. Rossky; Chem. Phys. Lett. 345, (2001) 159). We used molecular dynamics and tight-binding quantum chemical methods to compute the evolution of the electronic coupling. We explore the auto-correlation functions for the protein mediated electronic coupling and its decay time. We confirmed that the Franck-Condon approximation works well in ET for these Ruthenium-modified azurins.

Tustomu Kawatsu
Duke University

Date submitted: 11 Dec 2004 Electronic form version 1.4