



10th International Biophysics Congress
10^e Congrès international de biophysique

July / Juillet 29 - August / Août 3, 1990
Vancouver, Canada

Biophysics for the 90's
La biophysique pour les années 90

ABSTRACTS / RÉSUMÉS

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10TH INTERNATIONAL BIOPHYSICS CONGRESS

Vancouver Trade and Convention Centre
Canada Place, Vancouver
British Columbia, Canada
July 29 - August 3, 1990

Sponsored by:
Biophysical Society of Canada
National Research Council Canada
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RÉSUMÉS

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Vancouver Trade and Convention Centre
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S17.4 QUANTUM AND CLASSICAL ASPECTS OF ELECTRON TRANSFER REACTIONS: APPLICATION TO CHEMICAL AND BIOLOGICAL SYSTEMS. J.N.Onuchic, Department of Physics, University of California, San Diego, La Jolla, CA, USA, 92093, and Instituto de Física e Química de São Carlos, Universidade de São Paulo, São Carlos, SP, Brasil, 13560.

A theoretical discussion of electron transfer reaction will be presented. We will discuss why we believe that simple models work for these "complex" reactions. To build up a simple model we reduce the electronic part of the problem to a "two"-level system (reactants and products) which is coupled to the environment (nuclear modes or reaction coordinates). To do this a full separation into the important energy scales of the problem must be made. A discussion of the important time scales will be presented. Based on this we can separate the electronic part of the problem from the nuclear part as well as classify the nuclear motion. This analysis allow us to show why simple models are able to describe such obviously complex molecules. Using this framework we can describe strategies for numerical simulations that will provide parameters for these simple models.

Also, when building up the two-level system we have to calculate the electronic tunneling element that couples the two levels. We present calculations for these matrix elements for model compounds and Ru-modified proteins (myoglobin and cytochrome c). We show the tunneling "pathways" we believe dominate these matrix elements in specific protein.

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