Theoretical Studies Ranging from Quantum Dots to On-water Catalysis

By

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Biography:

Rudolph A. Marcus, Noyes Professor of Chemistry at the California Institute of Technology, was born in Montreal, Canada in 1923. He received a B.Sc. (1943) and Ph.D. (1946) from McGill University (experiment, Carl Winkler), followed by postdoctoral research with Edgar Steacie (experiment) and Oscar Rice (theory). He joined the faculty of the Polytechnic Institute of Brooklyn (1951-64), the University of Illinois (1964-78), and Caltech as Noyes Professor in 1978.

The Marcus theory of electron transfer processes and the RRKM theory of unimolecular reactions continue to be the standard theories in their fields. His pioneering contributions in other areas include vibrationally adiabatic reactions, reaction coordinate Hamiltonians, semiclassical collision theory, intramolecular dynamics, and "mass-independent" isotope effects in stratospheric ozone. The electron transfer theory has been applied to numerous fields and extended to atom, proton, and group transfers. His research is characterized by a strong interaction between theory and experiment and currently includes fluorescence intermittency of nanoparticles, single-molecule/ensemble studies of enzymes, on-water organic reactions, and unusual isotope effects in reactions.

His awards include the Nobel Prize in Chemistry (1992), the Wolf Prize in Chemistry (1985) and the National Medal of Science (1989).

Abstract:

With the advent of new experimental techniques, many experimental puzzles have arisen where theory plays a useful interactive and predictive role. Examples will be drawn from a broad range of recent studies by our group, such as the catalysis of certain organic 'on-water' reactions (green chemistry), the intermittent fluorescence of nanoparticles (quantum dots), fluctuations in single molecule properties of proteins, temperature independence of the H/D kinetic isotope effect for some enzymes operating under their natural conditions and an abnormal Arrhenius pre-exponential factor for a thermophilic enzyme operating below its break-point temperature, and a mass-independent isotope effect in ozone formation in the stratosphere.