Monday afternoon
Fifty Years of Electron Transfer and RRKM Theories
Ideas of Electron Transfer in Physical Chemistry
Cosponsored with HIST
S. J. Klippenstein and R. J. Cave, Organizers
A. A. Stuchebrukhov, Organizer, Presiding

1:20 — Introductory Remarks.

1:25 —162. Fifty-plus years of theory and running. R. A. Marcus

1:50 —163. Fifty years of the Marcus central dogma for electron transfer. J. Jortner

2:30 —164. Electron transfer theory: Some recent results in a retrospective aspect. A. M. Kuznetsov

3:10 — Intermission.

3:30 —165. Electron transfer mechanisms: Evolving theoretical probes and contact with experiment. M. D. Newton

4:10 —166. Finding reaction pathways in complex systems. D. Chandler

4:50 —167. Proton solvation and transport in aqueous and biomolecular systems. G. A. Voth

Tuesday morning

Fifty Years of Electron Transfer and RRKM Theories

Interaction with Experiment: Biological Electron Transfer

Cosponsored with HIST

A. A. Stuchebrukhov and S. J. Klippenstein, Organizers

R. J. Cave, Organizer, Presiding

8:00 —216. Electron tunneling through metalloproteins. H. B. Gray, J. R. Winkler

8:40 —217. DNA charge transport chemistry and biology. J. K. Barton

9:20 —218. Natural selection and variance in engineering electron tunneling networks and redox catalysis in photosynthesis and respiration. P. L. Dutton, C. C. Page, C. C. Moser

10:00 — Intermission.

10:20 —219. Structure-based electron transfer phenomena in proteins and DNA. M. E. Michel-Beyerle

11:00 —220. Structure-dependent electron tunneling mechanisms. D. N. Beratan

11:30 —221. Coupled electron transfer: Proton transfer reactions and proton pumping mechanism of cytochrome c oxidase. D. M. Popovic, A. A. Stuchebrukhov

Tuesday afternoon
Fifty Years of Electron Transfer and RRKM Theories
RRKM Theory and Experiment
Cosponsored with HIST
A. A. Stuchebrukhov and R. J. Cave, Organizers
S. J. Klippenstein, Organizer, Presiding

1:20 —253. A historical vignette: Mistakes our grandfather made. B. S. Rabinovitch

1:40 —254. Energy partitioning in unimolecular reactions: How good is the statistical theory? T. Baer, B. Sztáray

2:20 —255. Probing radical intermediates of bimolecular addition/insertion reactions. L. J. Butler, B. L. FitzPatrick, K -C. Lau, L. R. McCunn

2:40 —256. Mass independent isotope chemistry and the origin of the solar system, Mars and global climate change. M. H. Thiemens

3:20 — Intermission.

3:40 —257. An approximate theory for the isotopic effects of ozone formation. Y -Q. Gao

4:20 —258. Statistical theory of asteroid escape rates. C. Jaffé, S. D. Ross, M. W. Lo, J. Marsden, D. Farrelly, T. Uzer

4:40 —259. On modeling the pressure-dependent photoisomerization of trans-stilbene. J. R. Barker, R. E. Weston

Wednesday morning
Fifty Years of Electron Transfer and RRKM Theories
Applications and Extensions of Electron Transfer Theory
Cosponsored with HIST
A. A. Stuchebrukhov and S. J. Klippenstein, Organizers
R. J. Cave, Organizer, Presiding

8:00 —300. Energies governing electron transfer: What we know, what we need to learn. J. R. Miller

8:40 —301. Proton coupled electron transfer. T. J. Meyer, H. H. Thorp, M. H. Huynh

9:20 —302. From macroscopic to microscopic descriptions of electron transfer and proton transfer reactions: Quantifying Marcus parabolas. A. Warshel

10:00 — Intermission.

10:20 —303. Infrared-induced proton transfer in solution. J. T. Hynes

11:00 —304. Proton-coupled electron transfer: Couplings, rates, and isotope effects. S. Hammes-Schiffer

11:30 —305. An inhomogeneous model of proteins' dielectric response. X. Song

Wednesday afternoon
Fifty Years of Electron Transfer and RRKM Theories
Foundations of RRKM Theory
Cosponsored with HIST
A. A. Stuchebrukhov, S. J. Klippenstein, and R. J. Cave, Organizers
Y -Q. Gao, Presiding

1:20 —344. Uncertainties in calculating the RRKM unimolecular rate constant and remaining questions concerning unimolecular rate theory. W. L. Hase

2:00 —345. A new look at the transition state: Wigner's dynamical perspective revisited. C. Jaffé, S. Kawai, J. Palacián, P. Yanguas, T. Uzer

2:20 —346. IVR, RRKM and Coherent control. M. Gruebele

3:00 — Intermission.

3:20 —347. Influence of energy flow and localization on isomerization kinetics. D. M. Leitner

4:00 —348. Vibrational energy flow and non-adiabatic dynamics in gases and liquids. F. F. Crim

4:40 —349. Predicting rate constants for barrierless molecule-surface processes. O. J. Clarkin, D. M. Wardlaw

Thursday morning
Fifty Years of Electron Transfer and RRKM Theories
Interaction with Experiment: Molecular Electronics/Nanoscience
Cosponsored with HIST
S. J. Klippenstein and R. J. Cave, Organizers
A. A. Stuchebrukhov, Organizer, Presiding

8:00 —624. Electron transfer and molecular conductance: Some mechanistic issues. M. Ratner

8:40 —625. Electron transfer and molecular conduction. A. Nitzan

9:20 —626. Molecular currents in junctions and their fluctuations: A Louiville Space description. S. Mukamel, U. Harbola, M. Esposito, J. Maddox

10:00 — Intermission.

10:20 —627. Quantum dot blinking and power law electron transfer kinetics. V. Fomenko, D. J. Nesbitt

10:50 —628. Distance and angular dependence of long range electron transfer in peptides with different secondary structures. Y. Issa, K. Krogh-Jespersen, S. S. Isied

11:10 —629. Dynamics of electron spin transport as a function of temperature and electron spin-spin exchange coupling in a series of donor-bridge-acceptor para-phenylene oligomers. Z. E. X. Dance, D. McCamant, M. J. Ahrens, Q. Mi, M. A. Ratner, M. R. Wasielewski

11:30 —630. Electron and excitation transfer mediated by a midway molecule as an extension from Marcus's ET, and its realization in photosynthesis. H. Sumi

Thursday afternoon
Fifty Years of Electron Transfer and RRKM Theories
Theory of Reaction Dynamics
Cosponsored with HIST
A. A. Stuchebrukhov, S. J. Klippenstein, and R. J. Cave, Organizers
D. M. Wardlaw, Presiding

1:20 —672. Detailed SACM/CT treatment of the dissociation/recombination dynamics of hydrogen peroxide on an ab initio potential. J. Troe, V. Ushakov

2:00 —673. Exact quantum theory of chemical reactions and their resonances. A. Kuppermann

2:40 —674. Using the initial value representation (IVR) of semiclassical (SC) theory to describe electronically non-adiabatic processes in molecular systems. W. H. Miller

3:20 — Intermission.

3:40 —675. Imaging the dynamics of vibrational predissociation of hydrogen bonded complexes. G. Li, J. A. Parr, I. Fedorov, H. Reisler

4:00 —676. Dynamics of complex forming reactions C(3P,1D)+C2H2 -> C3+H2, l-C3H, c-C3H+H. J. M. Bowman, S. C. Park, C. Chen, B. J. Braams

4:40 —677. Applications of VTST in combustion chemistry: From methyl-methyl model to direct allyl-propargyl calculation. Y. Georgievskii

5:00 —678. Concluding Remarks. R. A. Marcus