Reading list, Chemistry 8565 – Chemical Reaction Dynamics

Reading for Monday, January 22, 2018
"Potential Energy Surfaces,"
D. G. Truhlar, in *The Encyclopedia of Physical Science and Technology*, 3rd edition, edited by R. A. Meyers (Academic Press, New York, 2001), Vol. 13, pages 9-17.
truhlar.chem.umn.edu/content/book-chapters-pdf-files

Reading for Friday, January 26, 2018
"An introduction to group theory for chemists"
J. E. White, J. Chem. Educ. **44**, 1280135 (1967).
doi.org/10.1021/ed044p128

Reading for Monday, January 29, 2018
"Relationships between E2 and E1cB mechanisms of β-elimination,"
R. A. More O'Ferrall, J. Chem. Soc. B, 1970, 274-277.
doi.org/10.1039/J29700000274

Reading for Friday, February 2, 2018
"Diatomic Molecules According to the Wave Mechanics. II. Vibrational Levels"
P M. Morse, Phys. Rev. 1929, 34, 57–64
doi.org/10.1103/PhysRev.34.57

Reading for Monday, February 5, 2018
"The Relative Likelihood of Encountering Conical Intersections and Avoided Intersections on the Potential Energy Surfaces of Polyatomic Molecules,"
D. G. Truhlar and C. A. Mead, Phys. Rev. A **68,** 32501/1-032501/2 (2003).
doi.org/10.1103/PhysRevA.68.032501

Reading for Friday, February 9, 2018
"Perspective on "Zur Quantentheorie der Molekeln","
J. C. Tully, Theor. Chem. Acc. **103**, 173-176 (2000).
doi.org/10.1007/s002149900049

Readings for Monday, February 12, 2018 (three readings)
"The Concept of Resonance,"
D. G. Truhlar, Journal of Chemical Education **84**, 781-782 (2007).
doi.org/10.1021/ed084p781
"Are Molecular Orbitals Delocalized?"
D. G. Truhlar, Journal of Chemical Education **89**, 573-574 (2012).
doi.org/10.1021/ed200565h
"Exploring the Nature of the H_2 Bond. 1. Using Spreadsheet Calculations To Examine the Valence Bond and Molecular Orbital Methods," Journal of Chemical Education **90**, 1452-1358 (2012).
A. M. Halpern and E. D. Glendening
doi.org/10.1021/ed400234g

Reading for Friday, February 16, 2018

"Nonadiabatic Transitions Between Ionic and Covalent States,"
R. K. Janev, Adv. At. Mol. Phys. **12**, 1-37 (1976). Read Sections I-III (pages 1-20).
doi.org//10.1016/S0065-2199(08)60041-X

Reading for Monday, February 19, 2018

"Chemical Equilibrium in Relation to Chemical Kinetics,"
K. Denbigh, in The *Principles of Chemical Equilibrium* (Cambridge University Press, 1955), Chaper 15.
https://ia800406.us.archive.org/30/items/ThePrinciplesOfChemicalEquilibrium/Denbigh-ThePrinciplesOfChemicalEquilibrium.pdf

Readings for Friday, February 23, 2018 (two readings)

"The Crossing of Potential Energy Surfaces,"
E. Teller, J. Phys. Chem. **41**, 109-116 (1937).
https://pubs.acs.org/doi/pdf/10.1021/j150379a010

"Internal Conversion in Polyatomic Molecules,"
E. Teller, Israel J. Chem. **7**, 227-236 (1969).
http://onlinelibrary.wiley.com/doi/10.1002/ijch.196900034/abstract (Read whole pdf.)

Reading for Monday, February 26, 2018

"Molecular Dynamics with Electronic Transitions,"
J. C. Tully, J. Chem. Phys. **93**, 1061-1071 (1990).
doi.org//10.1063/1.459170 (Read sections I–III and V.)

Readings for Friday, March 2, 2018 (two readings)

"Activated Complex Theory of Bimolecular Reactions,"
B. H. Mahan, Journal of Chemical Education **51**, 709-711 (1974).
dx.doi.org/10.1021/ed051p709

"Perspective on ``On the Theory of Oxidation-Reduction Reactions Involving Electron Transfer. I´´,"
J. M. Lluch, Theor. Chem. Acc. 103, 231-233 (2000).
https://link.springer.com/content/pdf/10.1007%2Fs002149900016.pdf

Readings for Monday, March 5, 2018 (three readings)

"Vignette: Electron Transfer Reactions,"
in *Physical Chemistry*, 2nd ed., edited by R. S. Berry, S. A. Rice, and J. Ross, Oxford University Press, New York, 2000), pp. 945-948.
https://comp.chem.umn.edu/courses/Marcus_Vignette.pdf

"Free Energy Surfaces for Liquid-Phase Reactions and Their Use to Study the Border Between Concerted and Nonconcerted α,β-Elimination Reactions of Esters and Thioesters,"
Y. Kim, J. R. Mohrig, and D. G. Truhlar, J. Am. Chem. Soc. **131**, 11071-11082 (2010).
dx.doi.org/10.1021/ja101104q (Read pages 11071-11074.)

"Chemical Kinetics and Mechanisms of Complex Systems: A Perspective on Recent Theoretical Advances,"
S. J. Klippenstein, V. Pande, and D. G. Truhlar, J. Am. Chem. Soc. **136**, 528-546 (2014).
dx.doi.org/10.1021/ja408723a