Readings for Chemistry 8565: "Chemical Reaction Dynamics"

Spring Semester 2023, two credits

Instructor: Donald G. Truhlar

Readings for Thursday, January 19:

1. "Potential Energy Surfaces," D. G. Truhlar, in *The Encyclopedia of Physical Science and Technology,* edited by R. A. Meyers (Academic Press, New York, 1987), 3rd ed. (2001), Vol. 13, pp. 9-17.

   Available online at https://comp.chem.umn.edu/Truhlar/docs/C27.pdf

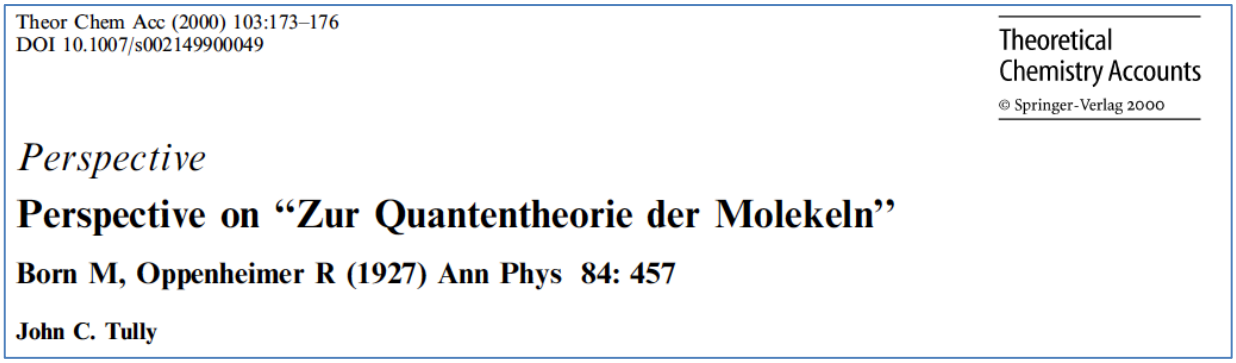
2. "Potential Energy Surfaces for Atom Transfer Reactions Involving Hydrogens and Halogens," C. A. Parr and D. G. Truhlar, Journal of Physical Chemistry **75**, 1844-1860 (1971). doi.org/10.1021/j100681a015

Readings for Tuesday, January 24:

1. "Dispersion Forces – Neither Fluctuating Nor Dispersing," D. G. Truhlar, Journal of Chemical Education **96**, 1671-1675 (2019). doi.org/10.1021/acs.jchemed.8b01044
   This J. Chem. Ed. paper is also available at
   https://truhlar.chem.umn.edu/courses/chemistry-8565-chemical-reaction-dynamics
2. "The Crossing of Potential Energy Surfaces,"
   E. Teller, J. Phys. Chem. **41**, 109-116 (1937).
   https://pubs.acs.org/doi/pdf/10.1021/j150379a010
3. "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.)
4. "Interaction of Vibrational and Electronic Motion in Alkali Halide Molecules," R. S. Berry, J. Chem. Phys. **27**, 1288 (1957).
5. "Collisional dissociation and chemical relaxation of alkali halide molecules: 2000–4200 K," R. Milstein and R. S. Berry, J. Chem. Phys. **80**, 6025 (1984).

Reading for Thursday, January 26:

Read the perspective article in *Theor. Chem. Acc.* by Tully about the Born-Oppenheimer paper and the Born-Oppenheimer approximation.



Theor Chem Acc (2000) 103:173–176
DOI 10.1007/s002149900049

Theoretical Chemistry Accounts

Perspective

Perspective on "Zur Quantentheorie der Molekeln"

Born M, Oppenheimer R (1927) Ann Phys 84: 457

John C. Tully

Reading for Tuesday, January 31:

Energy Contour Plots: Slices through the Potential Energy Surface That Simplify Quantum Mechanical Studies of Reacting Systems

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doi.org/10.1021/ed083p451

Reading for Tuesday, February 7:

JOURNAL OF CHEMICAL EDUCATION Article
pubs.acs.org/jchemeduc

Exploring the Nature of the H_2 Bond. 1. Using Spreadsheet Calculations To Examine the Valence Bond and Molecular Orbital Methods

Arthur M. Halpern* and Eric D. Glendening

doi.org/10.1021/ed400234g | *J. Chem. Educ.* **2013**, *90*, 1452−1458

Reading for Tuesday, February 14:
https://truhlar.chem.umn.edu/sites/truhlar.chem.umn.edu/files/files/denbigh_-_chapter_15.pdf

Readings for Thursday, February 16:
"Potential energy surface for H_3" R. N. Porter and M. Karplus, Journal of Chemical Physics **40**, 1105-1115 (1964). doi.org/10.1063/1.1725256

"Thermodynamic Calculations," M. Randall, J. Chem. Educ. **8**, 1062-1073 (1931).

Reading for Tuesday, February 21:
Eyring, H. (1938). The theory of absolute reaction rates. Transactions of the Faraday Society, 34, 41-48. doi:10.1039/TF9383400041

Readings for **Thursday, February 21:**

Wigner, E. The Transition State Method. Transactions of the Faraday Society, 34, 29-41 (1938). doi: 10.1039/TF9383400029

C. N. Hinshelwood et al., General Discussion. Transactions of the Faraday Society, 34, 70-81 (1938). doi: 10.1039/TF9383400070

Readings for **Thursday, March 2:**

"Transition State Theory," B. C. Garrett and D. G. Truhlar, in *Encyclopedia of Computational Chemistry*, edited by P. v. R. Schleyer, N. L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, and H. F. Schaefer III (John Wiley & Sons, Chichester, UK, 1998), Volume 5, pp. 3094-3104. https://comp.chem.umn.edu/Truhlar/docs/C58.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 (Especially 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, Journal of the American Chemical Society **136**, 528-546 (2014). doi.org/10.1021/ja408723a