Schrödinger

Workshop #2 for Educator's Week 2026

Mapping the Reaction "Mountain Pass": Visualizing Transition States with Schrödinger's AutoTS Panel

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Education Team

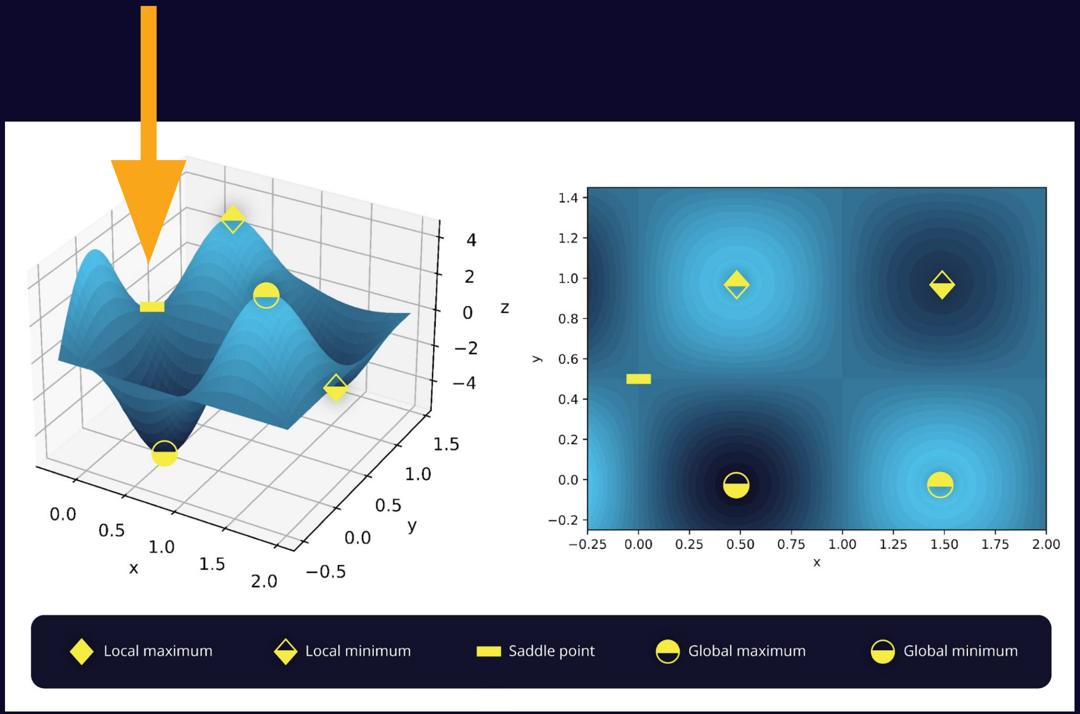
Workshop Learning Objectives

1. **Bridge the Abstract-to-Concrete Gap: Visualizing Reaction Coordinates**
   - Use Jaguar animations to transform the Transition State from a 2D graph into a tangible 3D physical structure
   - Connect the Potential Energy Surface "hump" to actual atomic movement, illustrating how bonds break and form
2. **Facilitate Inquiry-Based Learning: The "In Silico" Experiment**
   - Use AutoTS labs to let students map reactant-to-product transitions and test their own mechanistic hypotheses
   - Teach students to use computational data, specifically activation energy ($\Delta G^{\ddagger}$), to justify their chosen reaction mechanisms
3. **Evidence-Based Reasoning: Proving Hammond's Postulate**
   - Use computational TS geometries to "prove" Hammond's Postulate by measuring bond lengths, shifting students from rote memorization to evidence-based justification

Hands-on Demo

What is a transition state?

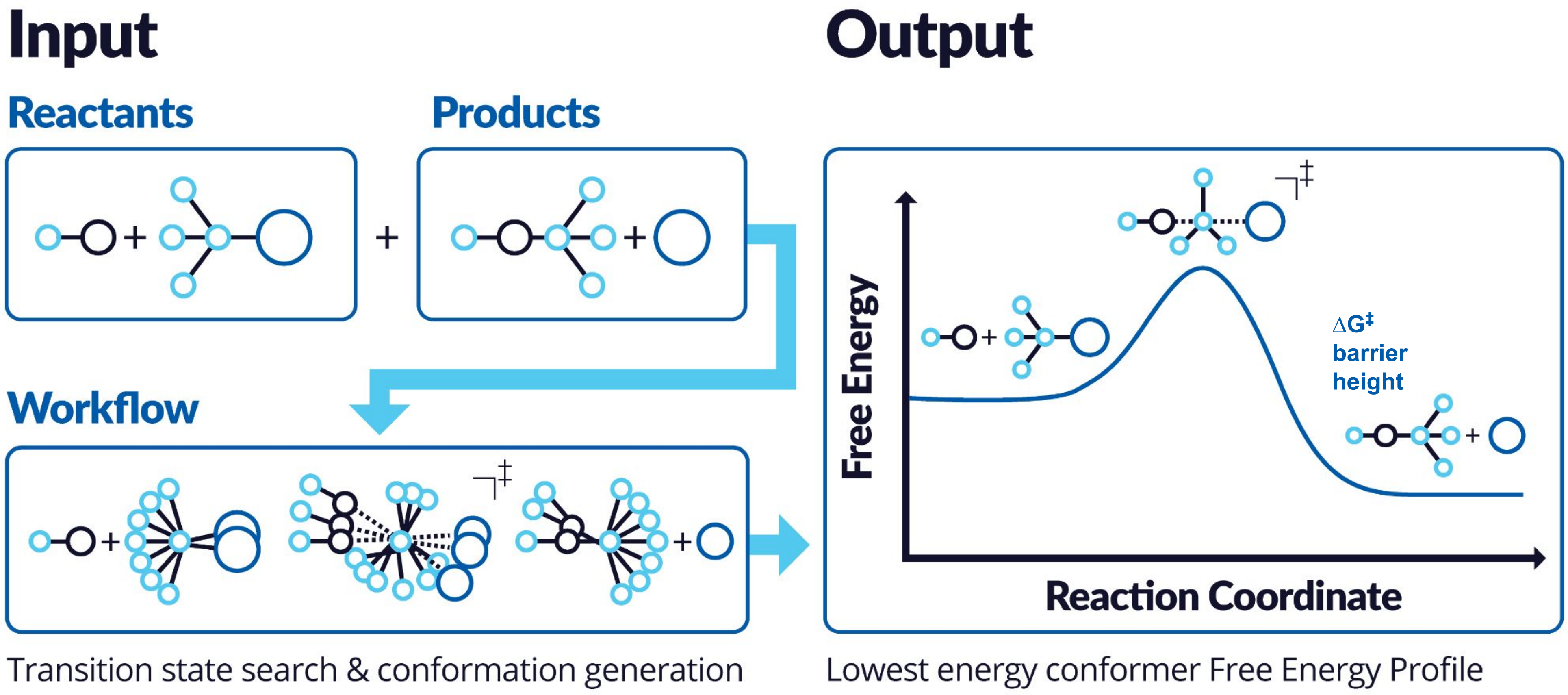
- The transition state corresponds to a first-order saddle point on the potential energy surface (PES) that describes a reaction with an energetic barrier.
- Locating a transition state is essential for computing the activation energy of a reaction and thereby the rate.
- Finding transition states is useful in many materials science applications, including:
  - Predicting reactivity
  - Understanding reaction mechanisms
  - Catalyst design and optimization
  - Predicting outcomes of various competing reactions
- Since transition states are momentary, they can only be studied computationally.



Locating Transition States: Part 1
Example: Diels-Alder reaction

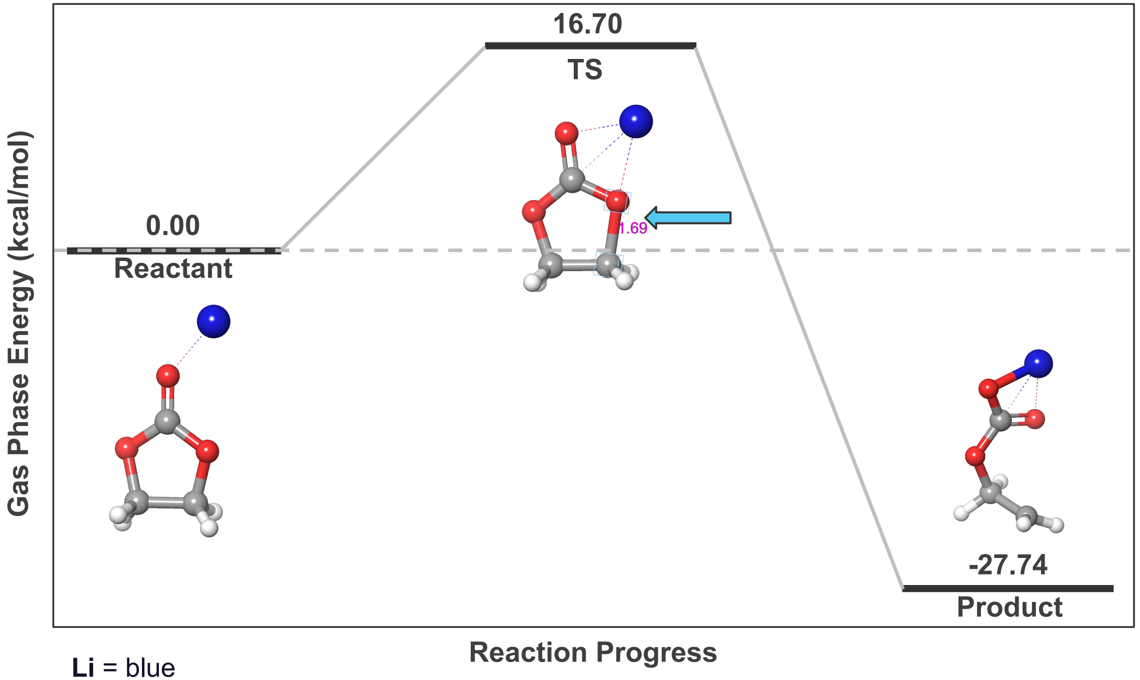
AutoTS: automated transition state searching

Automated workflow for optimizing transition states of elementary reactions, conformational search and post-processing



Reaction mechanism of C-O bond breaking

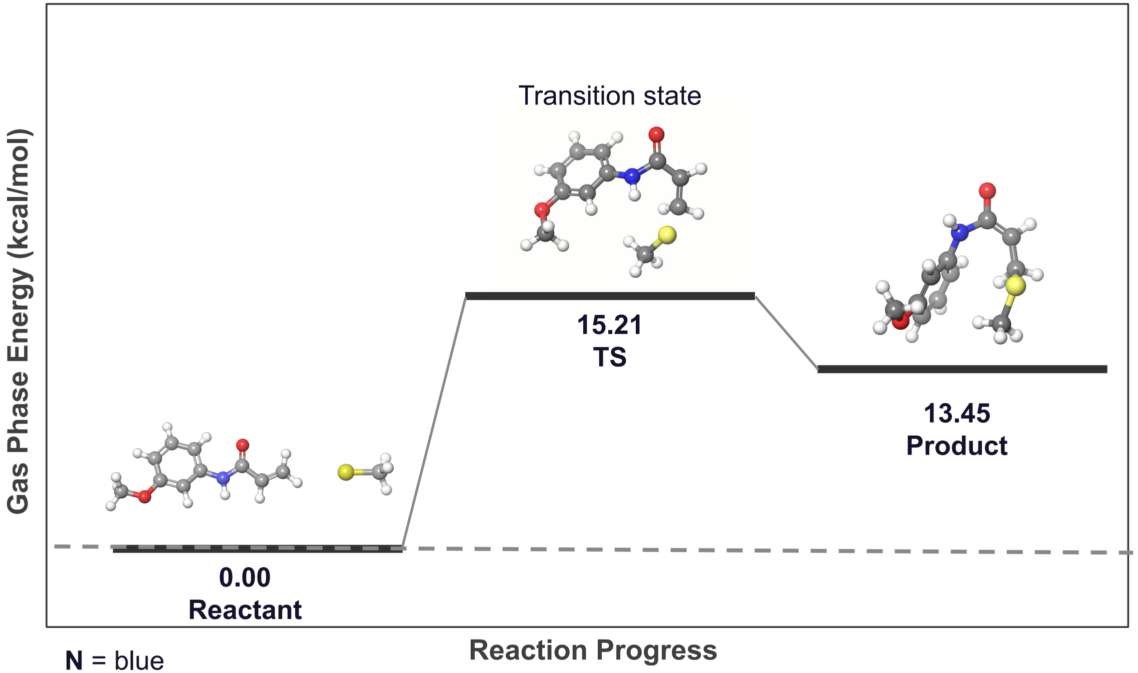
Exothermic



Li = blue
O = red
C = grey
H = white

Michael addition reaction mechanism

Endothermic



N = blue
O = red
C = grey
H = white
S = yellow

Classroom Exercise Suggestions

1. **Exercise 1: Hammond's Postulate Lab**
   - Does the Transition State (TS) look more like the "Before" (Reactants) or the "After" (Products)?
   - ***Task:*** Measure the lengths of the breaking and forming bonds in the TS structure using the Measure Tool
   - ***Data to collect:*** Compare these lengths to the bond distances in the starting materials and final products
   - ***Main takeaway:*** Use your measurements to prove if the reaction is Exothermic (Early TS) or Endothermic (Late TS)

2. **Exercise 2: The "Imaginary" Vibration Challenge**
   - A Transition State is a "Saddle Point"—the highest point on the path between two valleys
   - ***Task:*** Open the Vibrational Analysis tab and locate the single negative (imaginary) frequency
   - ***Data to collect:*** Click "Animate" and watch how the atoms move. Compare this to a "normal" positive frequency
   - ***Main takeaway:*** Explain why only the negative frequency shows the "pathway" to the product while others just show the molecule "stretching"

Alignment to Student Learning Outcomes from the American Chemical Society (ACS) Guidelines

1. Foundational & In-Depth Concepts: Kinetics and Mechanisms

- **ACS Requirement:** Students must understand the "molecular-level details of chemical reactions, including rate laws, collision theory, and reaction mechanisms"
- **Workshop Alignment:** By using AutoTS, students move beyond 2D "arrow pushing" to see the precise 3D geometry of a transition state
- **Student Learning Outcome:** Students will be able to distinguish between a transition state (a saddle point) and an intermediate (a local minimum) by analyzing the vibrational frequencies and the potential energy surface

2. Computational Chemistry & Molecular Modeling (Section 5.4)

- **ACS Requirement:** Programs must provide students with experience in "computational chemistry and molecular modeling"
- **Workshop Alignment:** This workshop provides a "Guided Discovery" model where students use industry-standard software (Maestro/Jaguar) to calculate energies, optimize structures, and visualize molecular orbitals or interaction maps
- **Student Outcome:** Students demonstrate "Computational Literacy" by performing iterative design cycles and using scoring functions to evaluate chemical hypotheses

Thank you for attending!

Please join us for another workshop this week:

- **Searching for the "Chemical Core" using Ligand-Based Virtual Screening with Phase**: Thurs. April 30th from 11-11:30am ET
  - Recommended for educators teaching biochemistry, medicinal chemistry

We will email today's workshop materials so you can walk through the same steps on your own.

For any questions, please reach out to teaching@schrodinger.com