Potential Energy Surfaces for Excited States of CH_2I_2

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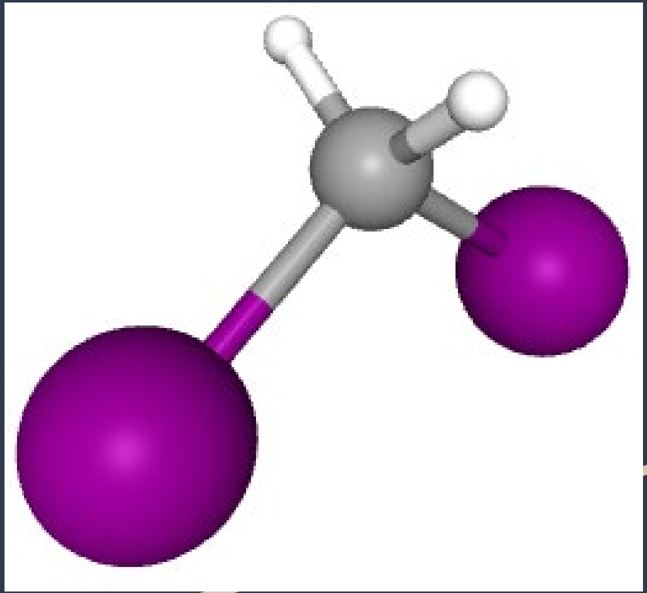
2023 Kansas State University Physics REU

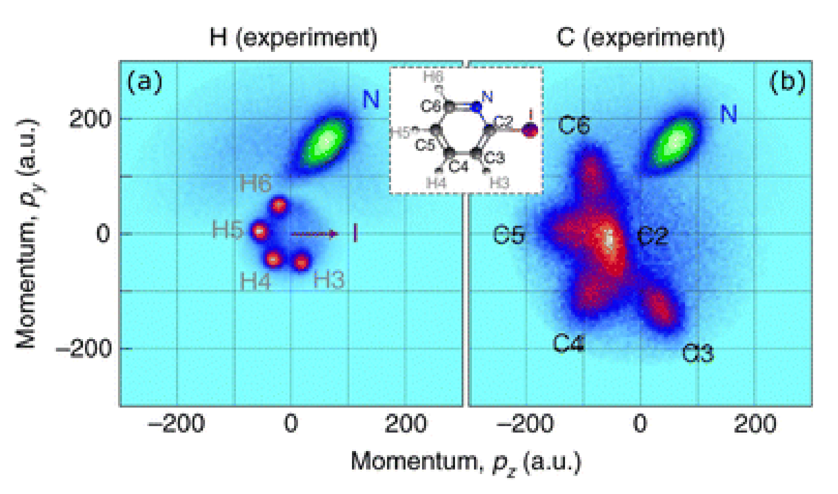
Coulomb Explosion



Pubchem:
https://pubchem.ncbi.nlm.nih.gov/compound/diiodomethane#section=3D-Conformer

- This method investigates molecules, like CH_2I_2, by breaking them.
- In this case, a “pump” photon with a wavelength of 200 nanometers excites the molecule.
- An infrared “probe” breaks the molecule.
- The pieces are examined.

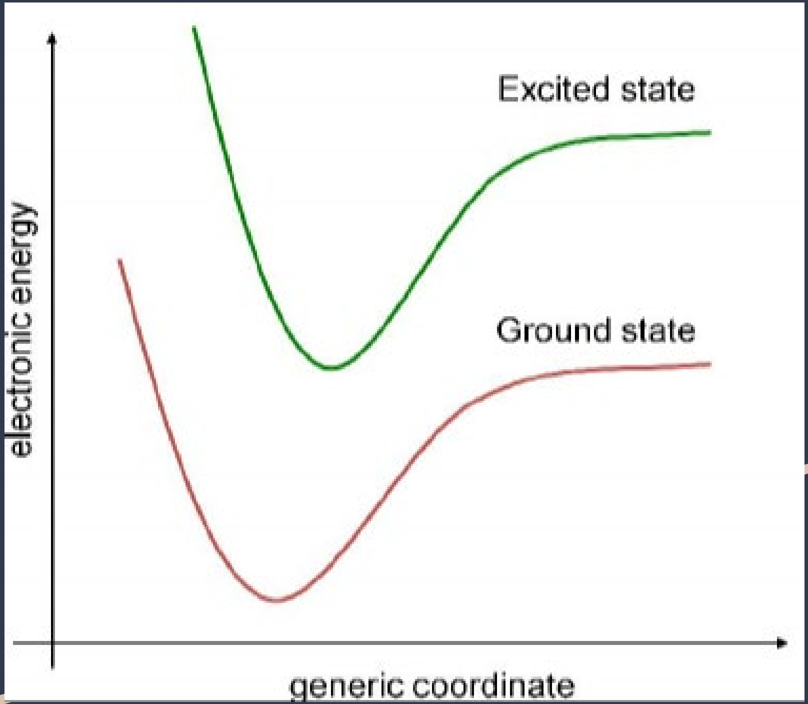
Theory Connection



Crane, et al. Phys. Chem. Chem. Phys. 25 (2023)

- Coulomb Explosion Imaging looks at the products.
- The theorist tries to match models to the experimental results.
    - How do the results come about?
- My project was to describe the excited state dynamics of CH_2I_2.

Potential Curves



Ullah, H. (2015) Density Functional Theory Study of Electronic and Structural Properties of Polyaniline and Poly(o-Phenylinediamine) Oligomers.

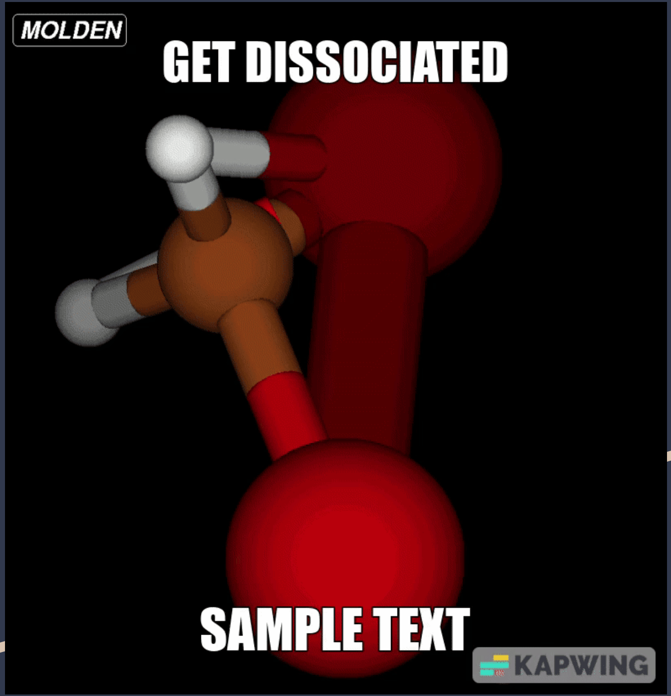
- A geometric parameter is plotted against potential energy.
- The bond is at equilibrium at the lowest point.
- Excited states can have different equilibrium bond lengths, or be unbound.

Schrödinger Equation

$$E\Psi = H\Psi$$
$$E\Psi = (kinetic + potential)\Psi$$
$$E\Psi = (\Sigma p^2/2m_e + \Sigma q_1 q_2/r^2)\Psi$$

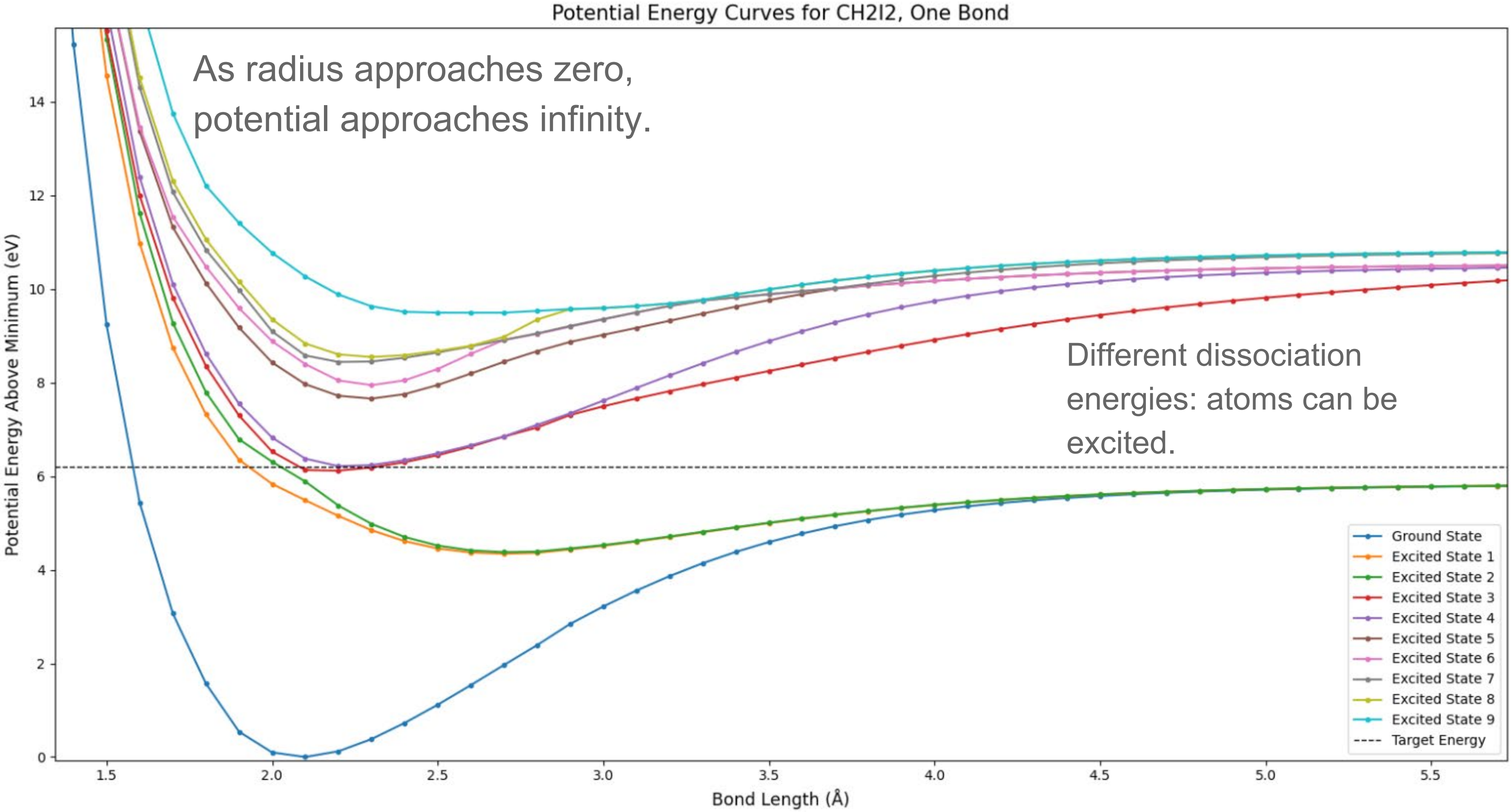
- Solving the molecular Schrödinger equation.
- The potential term is a Coulomb potential.

The Process

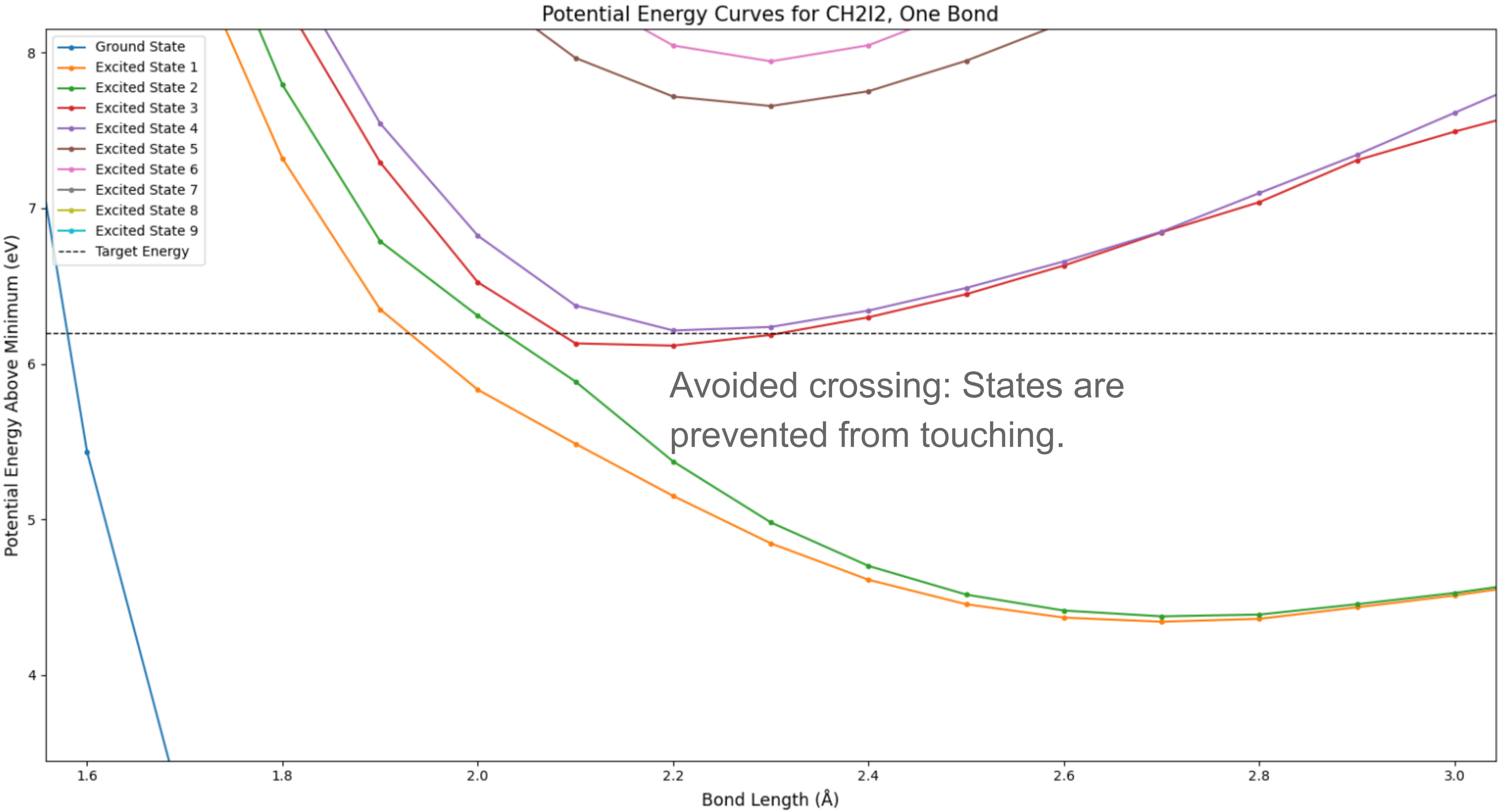


- Molpro solves the equation!
- Fed the geometry into Molpro to optimize electron orbitals and potential.
- Varied the geometry to make a curve.
  - Changed bond lengths.
- Increased the number of excited states in Molpro.

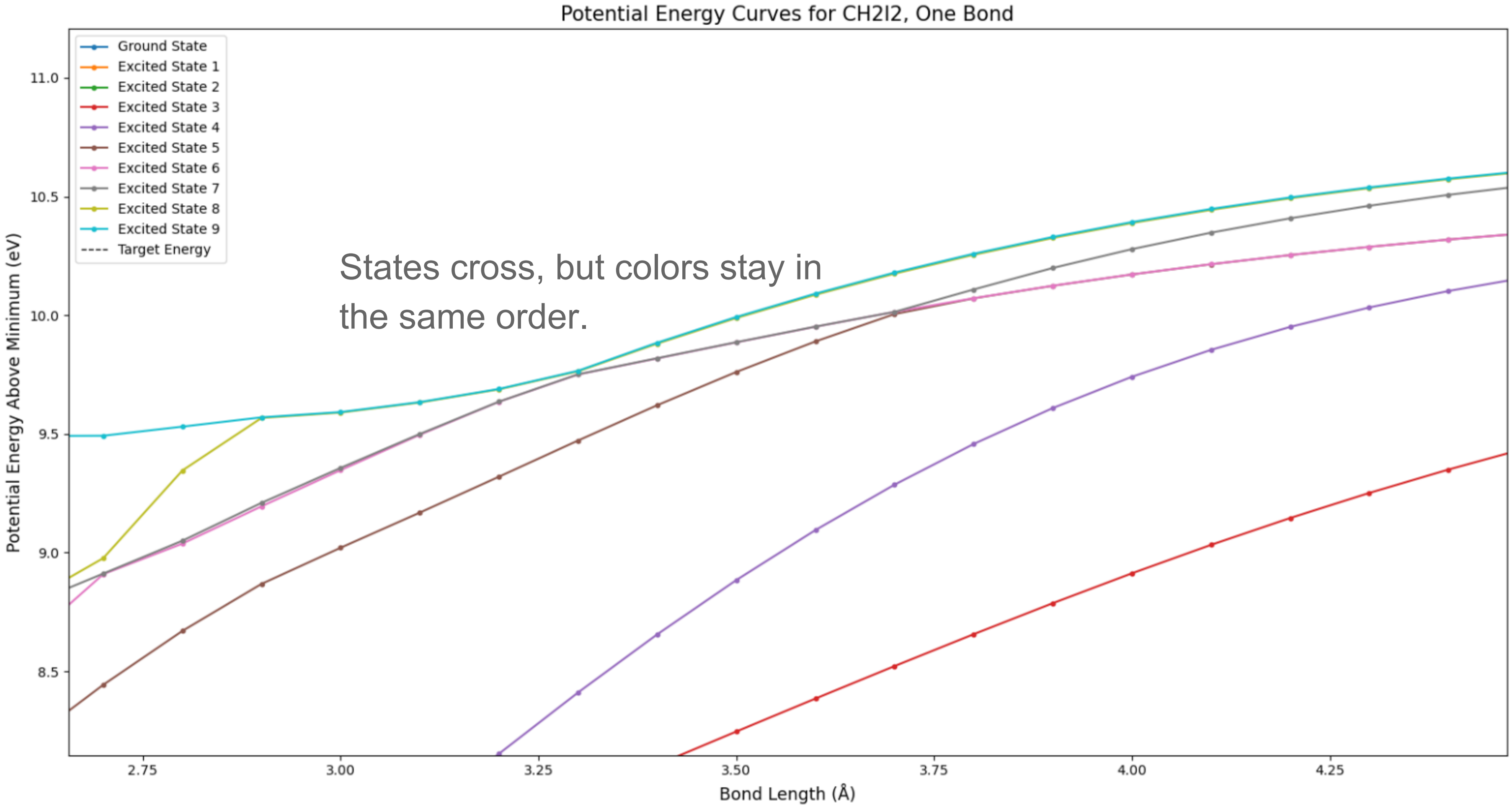
Results: One Bond



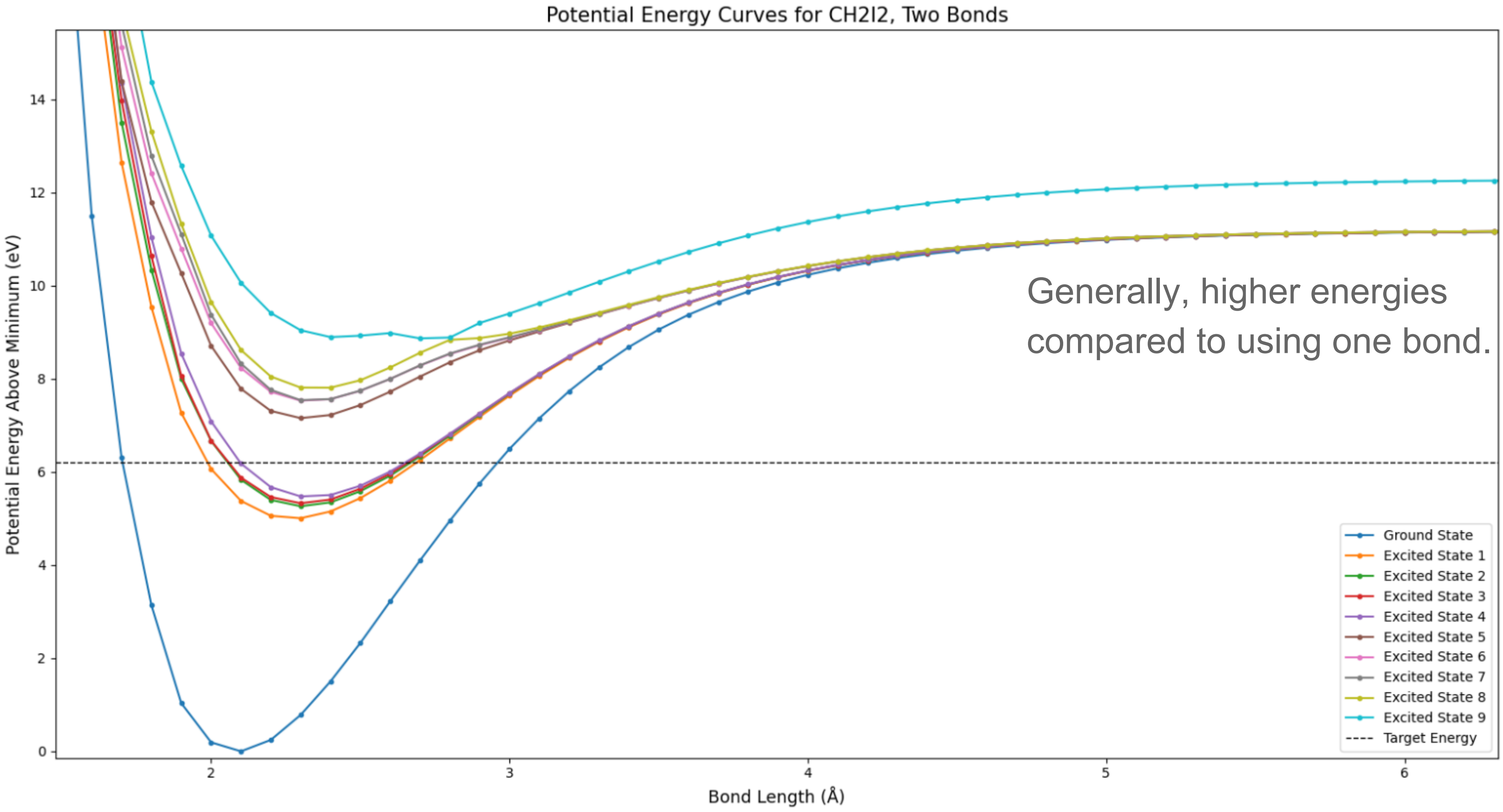
Results: One Bond



Results: One Bond

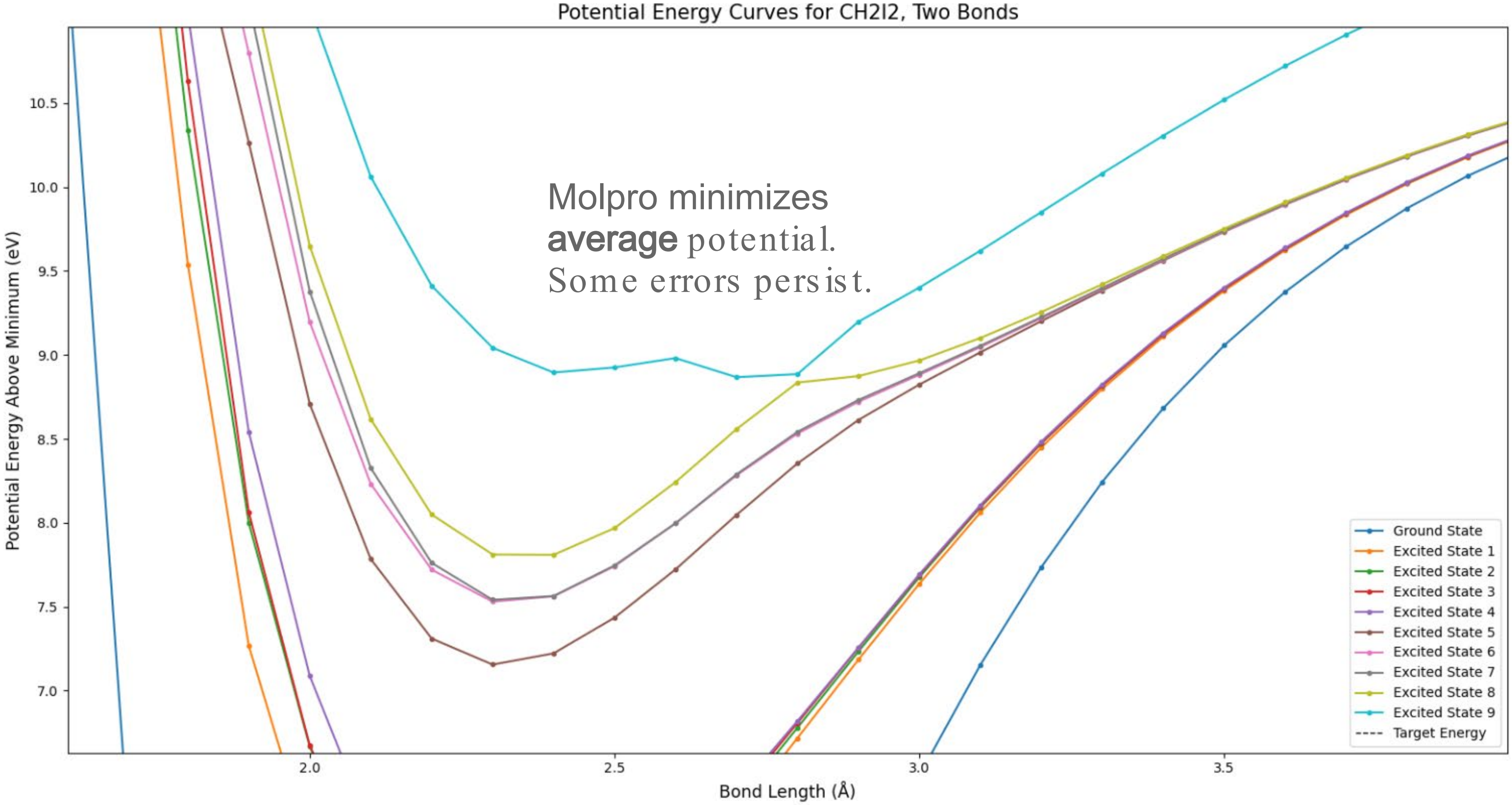


Results: Two Bonds



Generally, higher energies compared to using one bond.

Results: Two Bonds

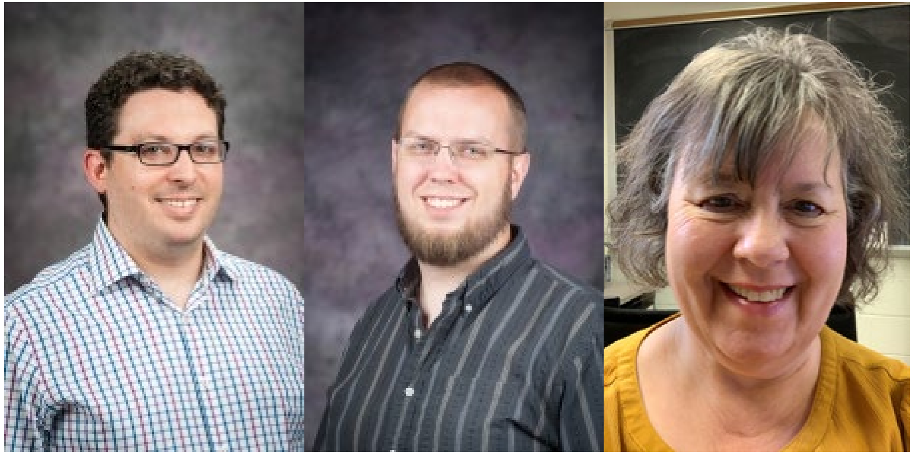


Molpro minimizes **average** potential. Some errors persist.

In Summary…

- The goal of this research was to characterize the excited states of CH_2I_2, up to an energy of 200 nm.
- This was accomplished by the creation of potential energy surfaces.
- Bond lengths were varied, and the minimum possible potential was recorded for each length.

Acknowledgements



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Any Questions?