Synchrotron Photoionization Mass Spectrometry for Investigation of Combustion Chemistry

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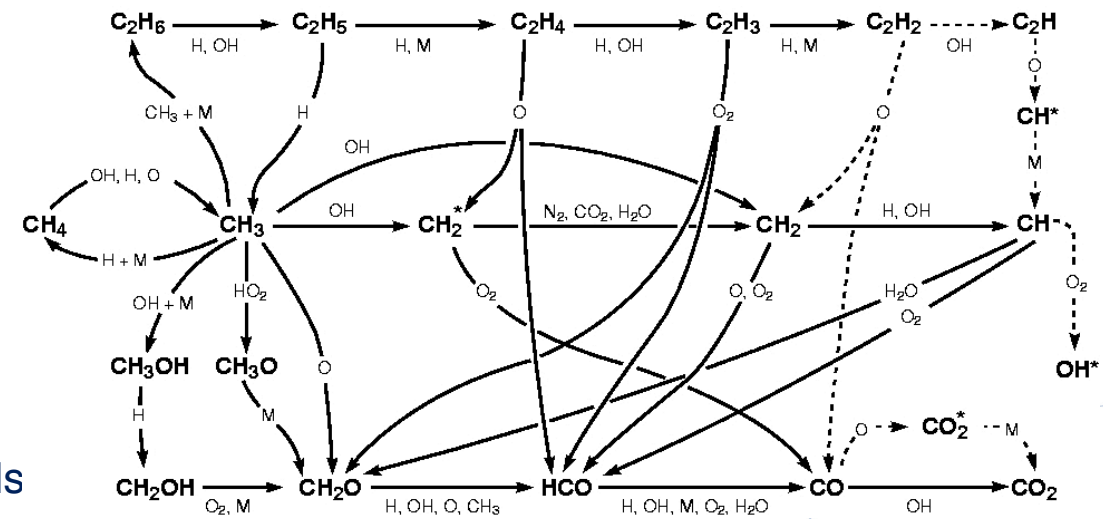
Introduction

- ✓ 85 % of the energy consumed in the U.S. is produced by Combustion Processes

- ✓ For even the simplest fuels (e.g. methane), the chemistry of combustion consists of hundreds of reactions

  Real fuels (e.g. gasoline) contain hundreds of compounds

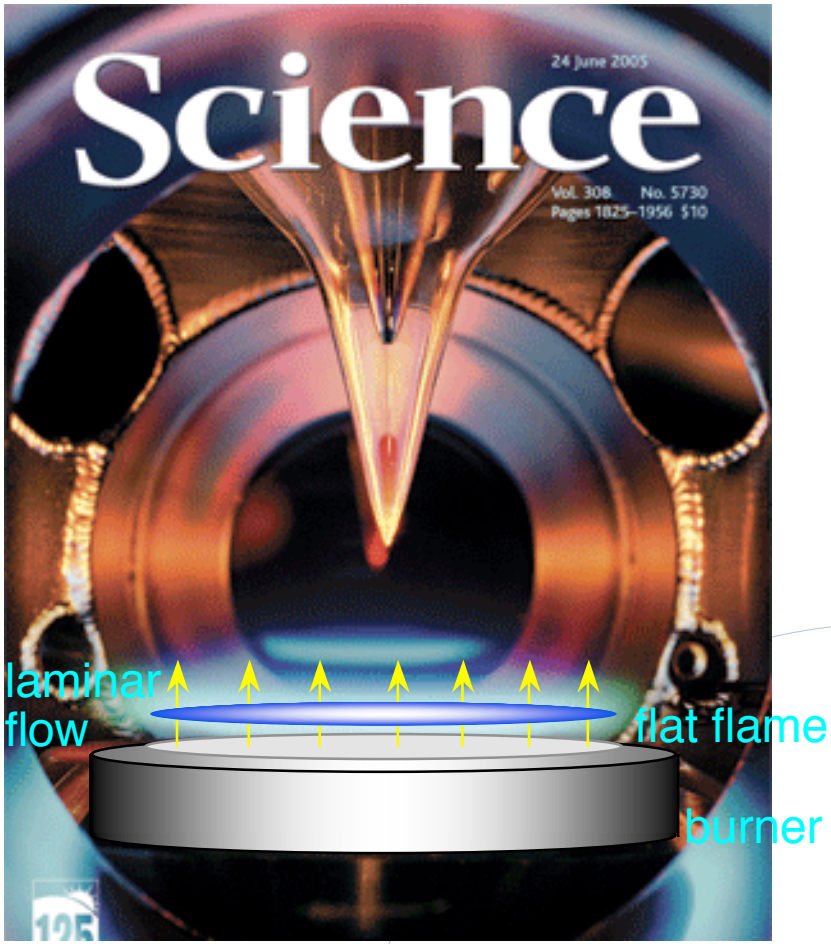


- ✓ Details matter for ignition, pollutant production, soot formation

- ✓ Methods for observing key reaction species in combustion environments are required

1D Laminar Low-Pressure Flames - A Test Case for Kinetic Mechanisms

- ✓ Identification of a wide range of species
  - ➢ by mass
  - ➢ by ionization energy
- ✓ Mole fraction profiles of stable species and radicals
  - ➢ axially resolved
  - ➢ comparison with flame model predictions



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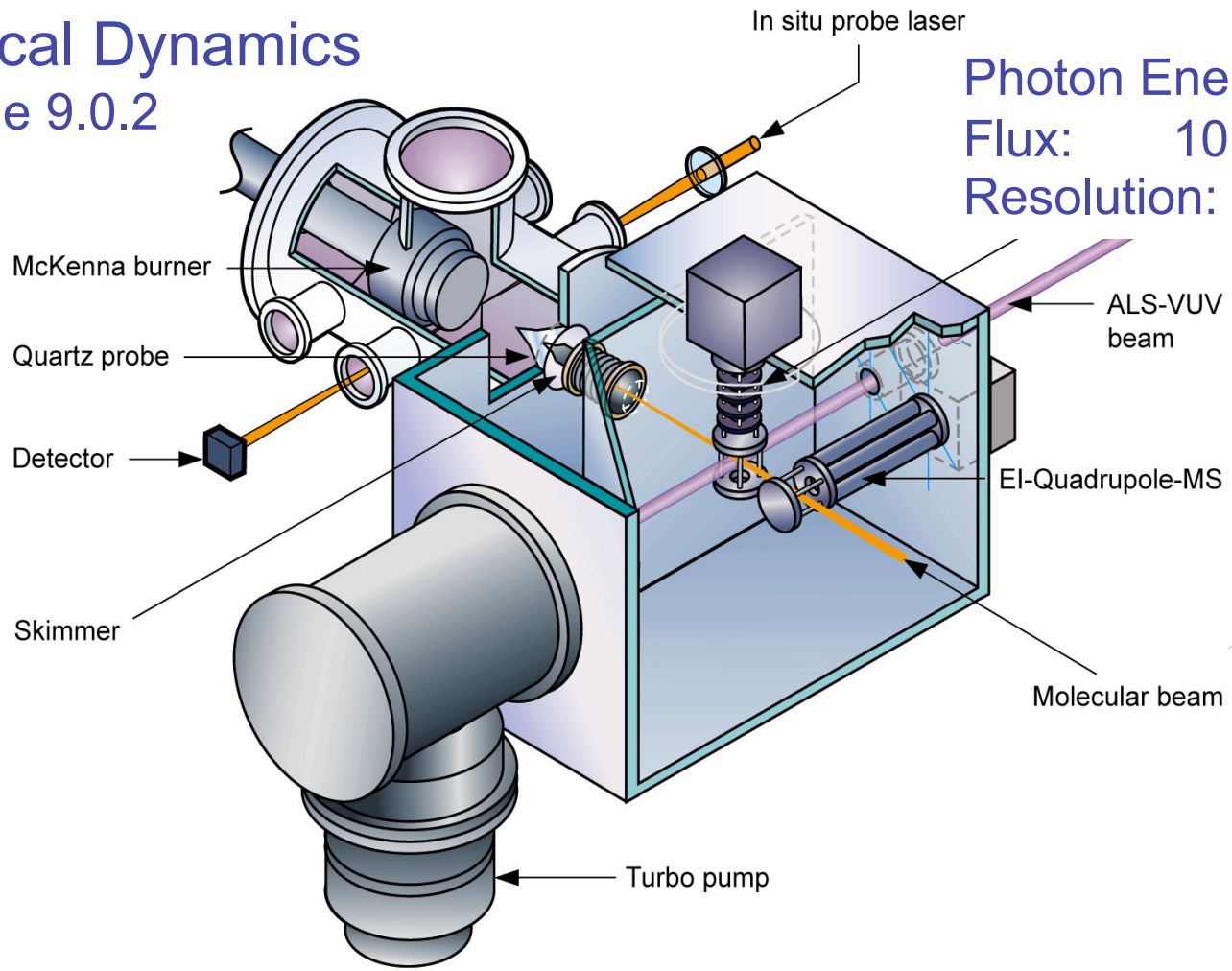
Flame Machine at the Advanced Light Source: Photoionization Mass Spectrometry

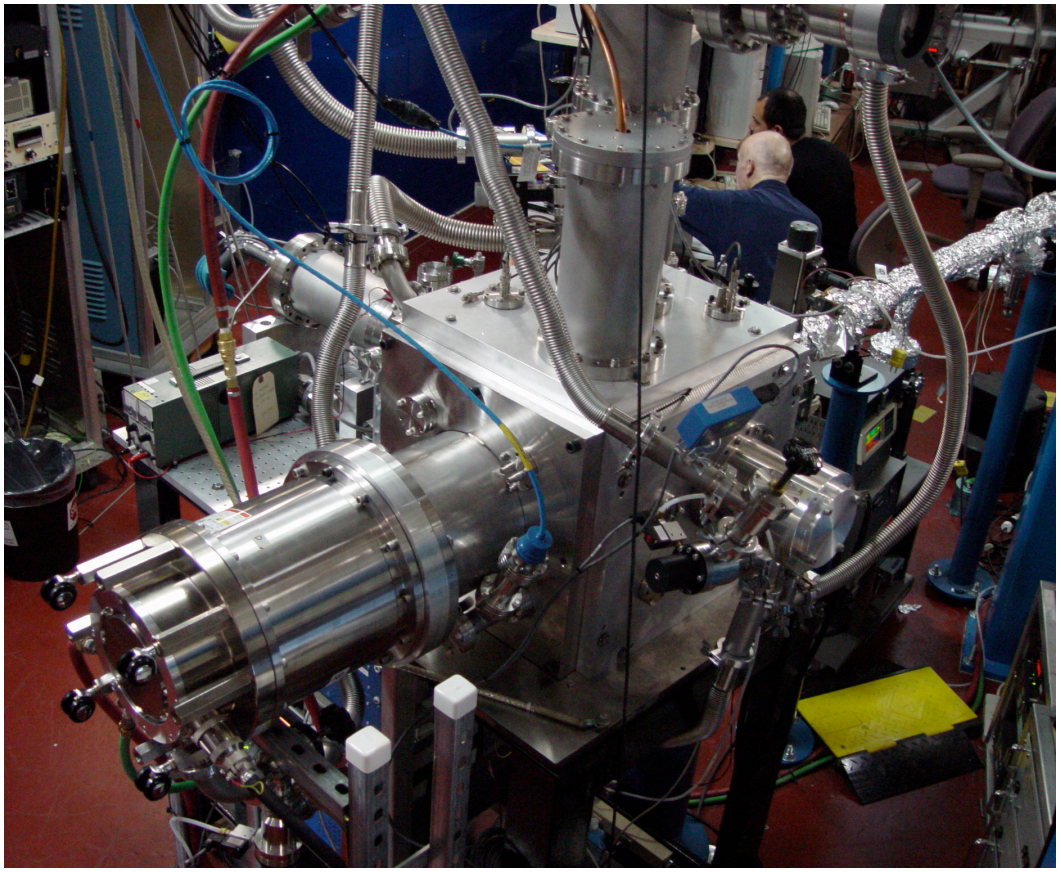
Chemical Dynamics

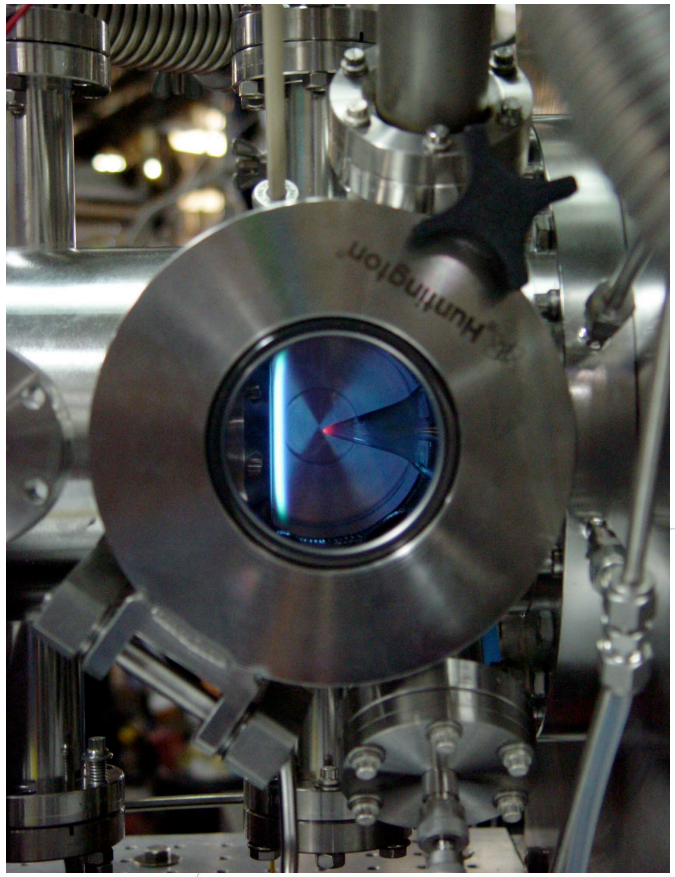
Beamline 9.0.2

Photon Energy: 7-24 eV
Flux: 10^{11} photons/s
Resolution: $E/\Delta E = 400$

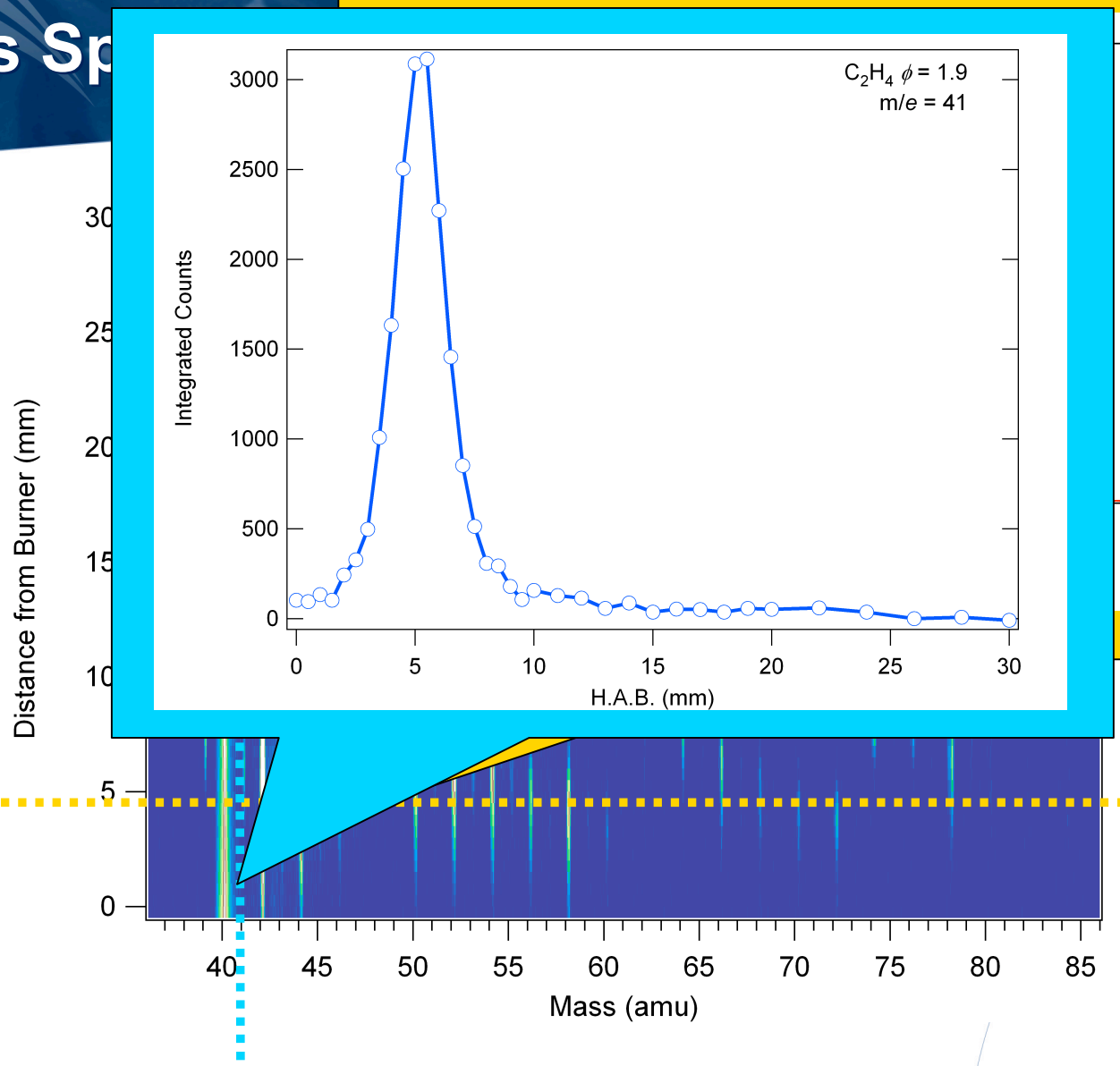


Flame Machine at the Advanced Light Source: Photoionization Mass Spectrometry

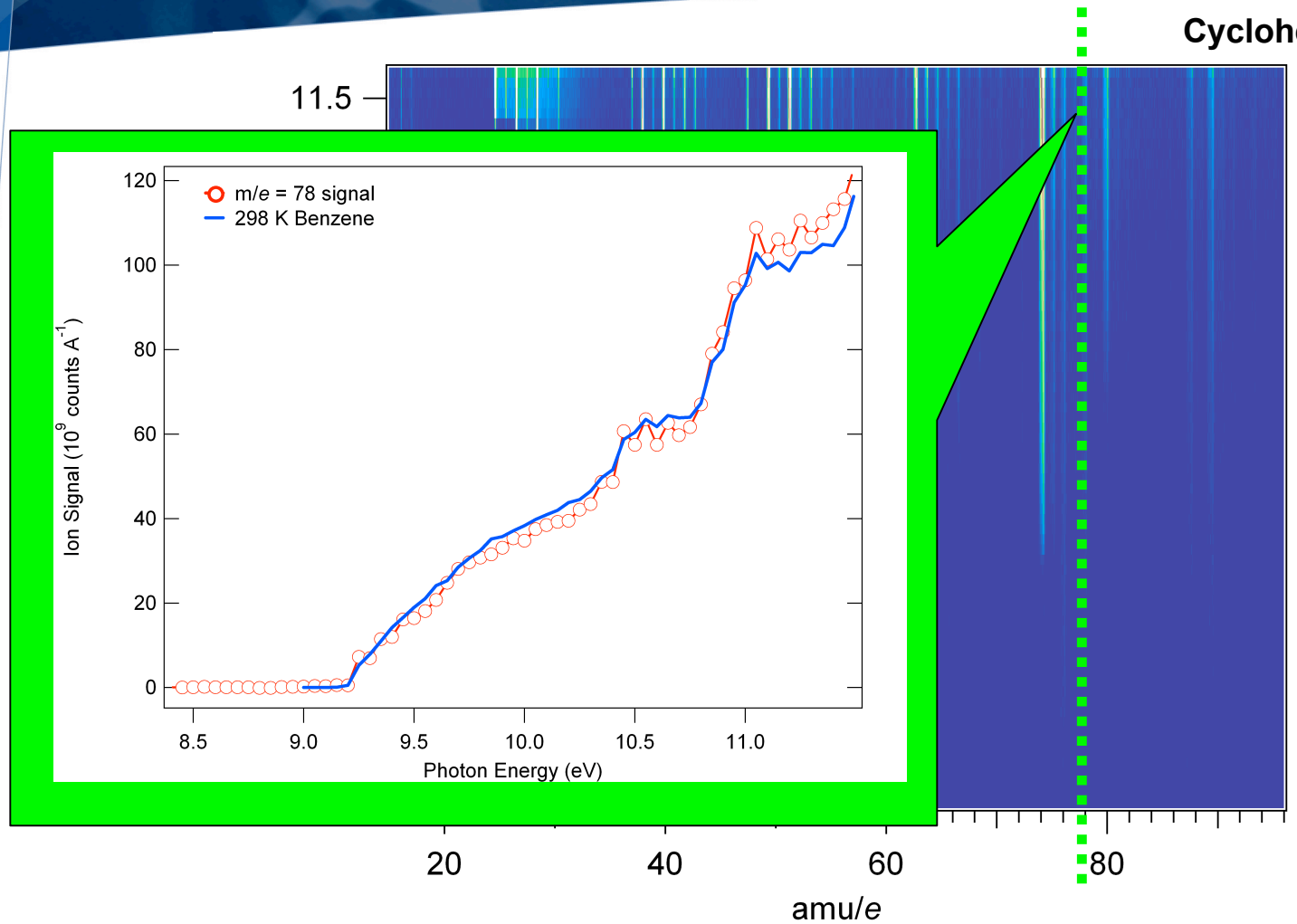




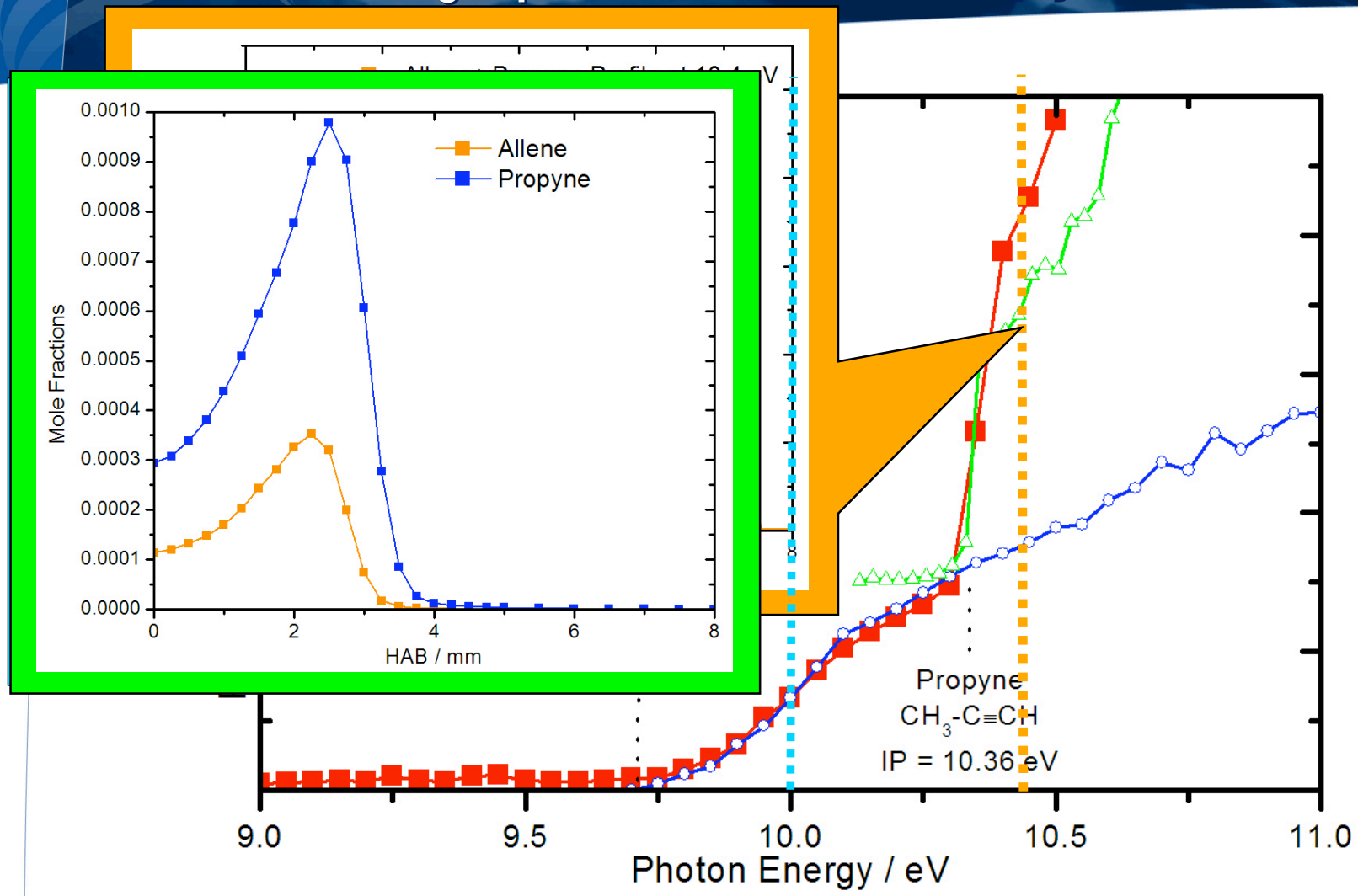
Burner Scan: Mass Sp



Energy Scan: Photoionization Efficiency Curves and Identification



Energy Resolution of ALS Can Resolve Isomers – C_3H_4: Allene and Propyne



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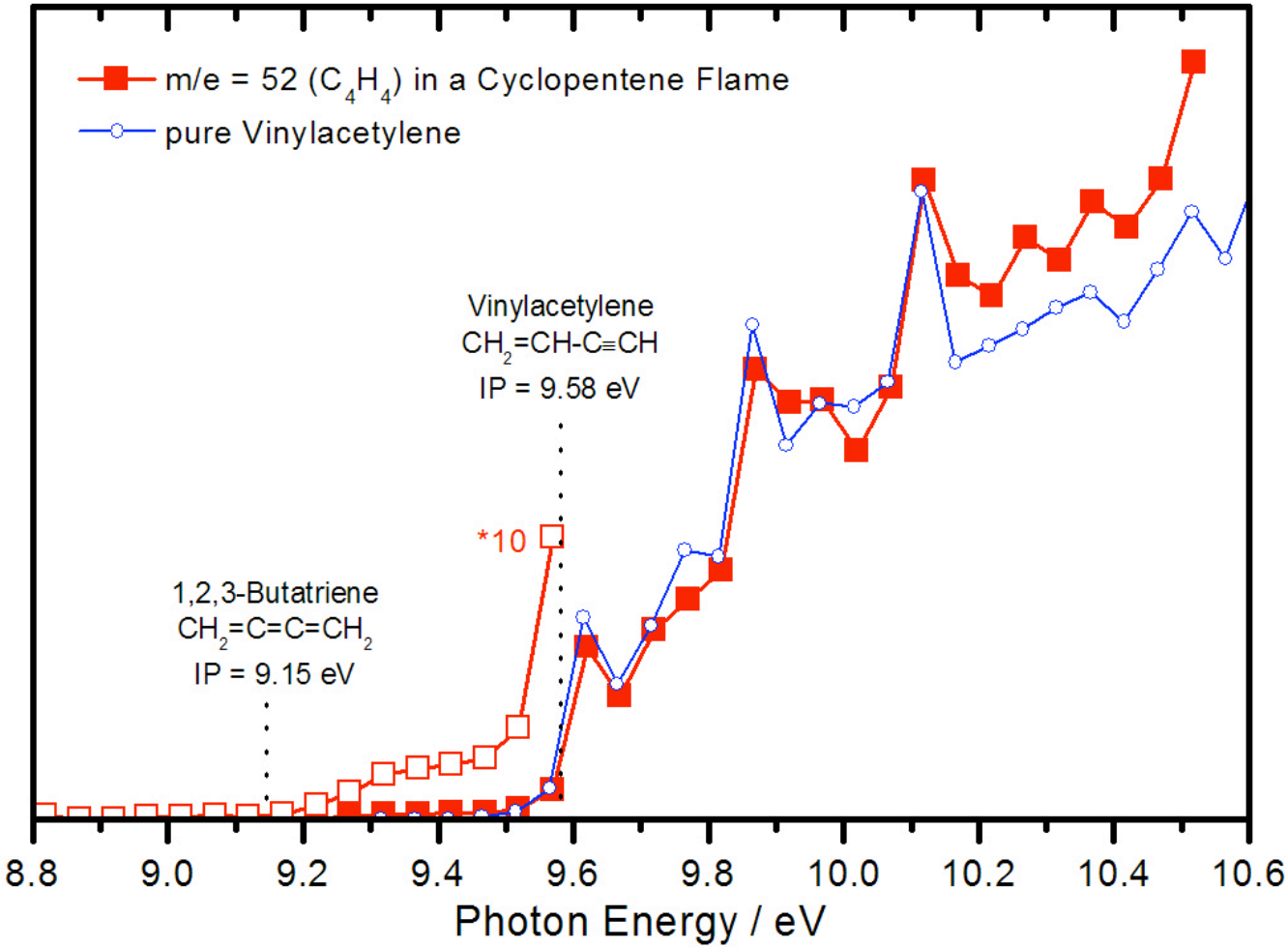
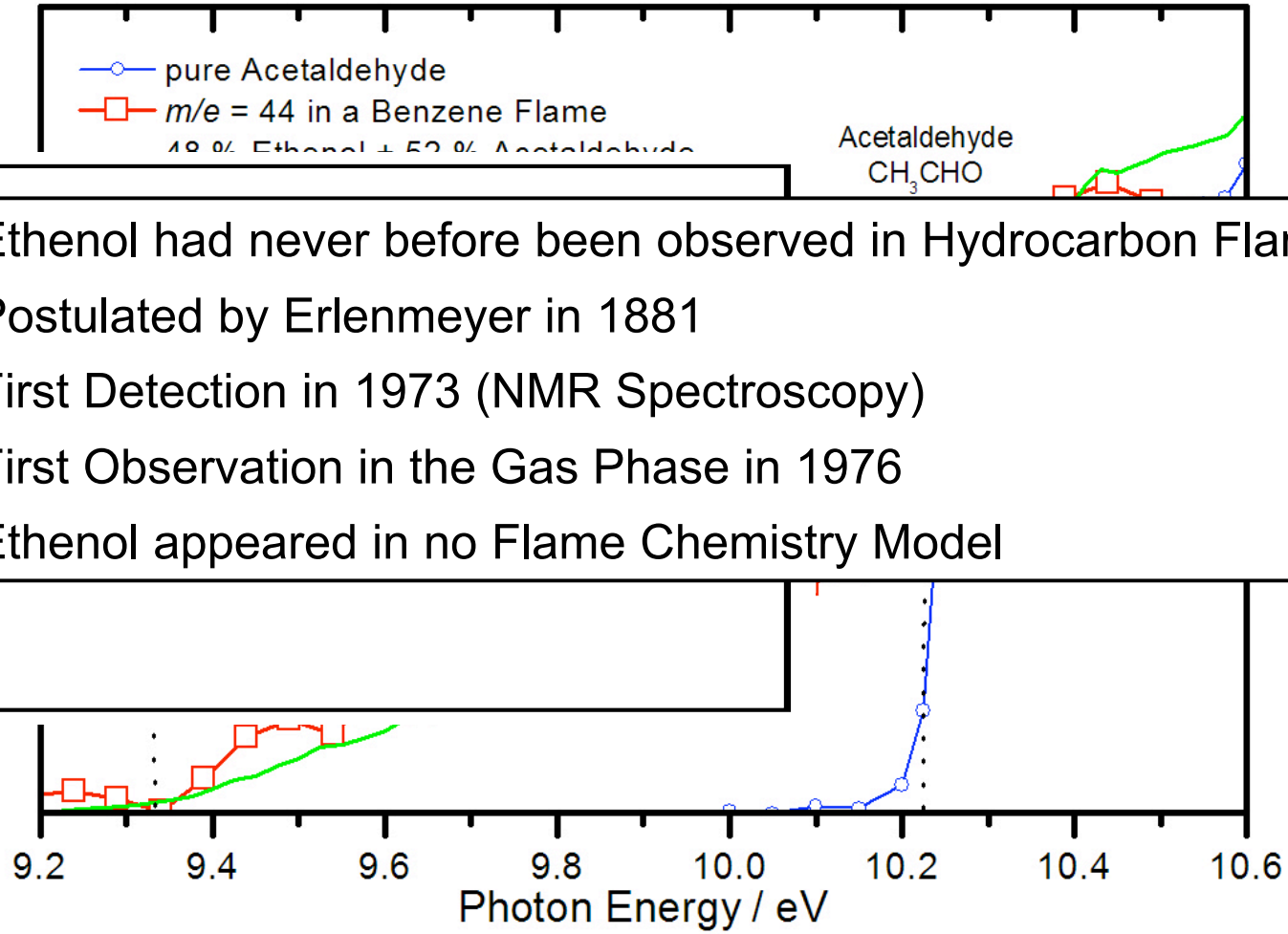
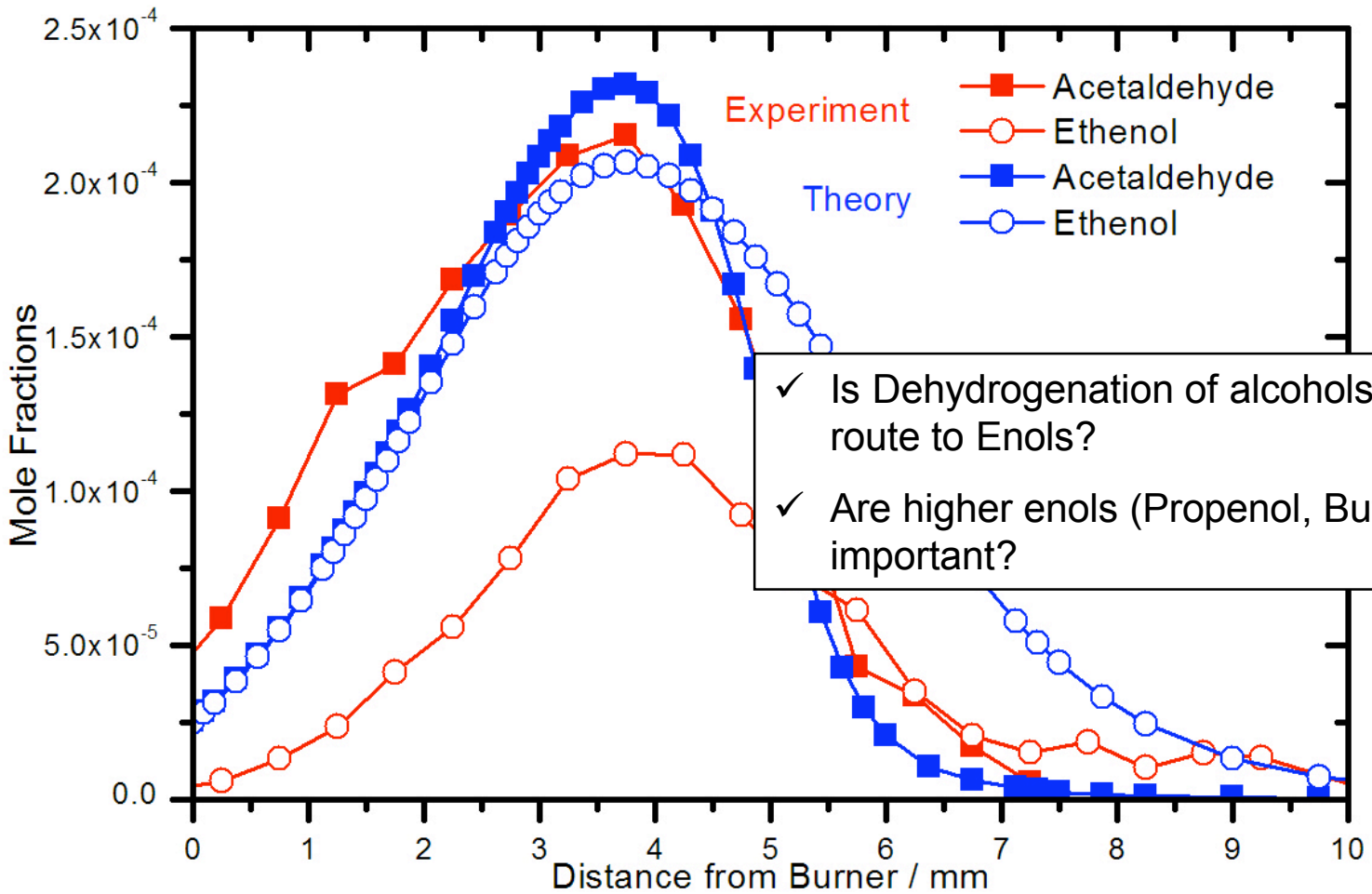


Detection of Ethenol (Vinylalcohol) – an Isomeric Form of Acetaldehyde



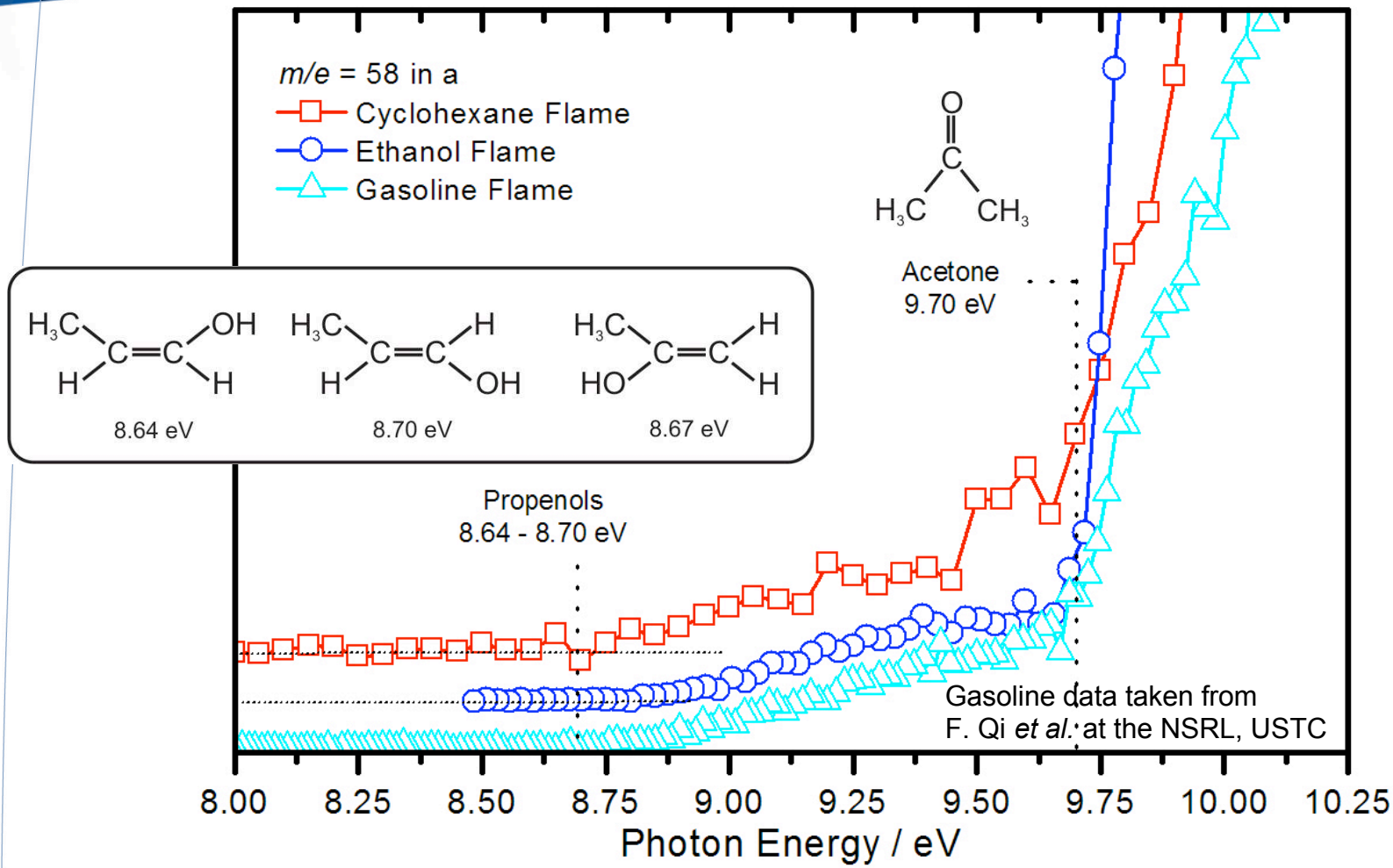
- Ethenol had never before been observed in Hydrocarbon Flames
- Postulated by Erlenmeyer in 1881
- First Detection in 1973 (NMR Spectroscopy)
- First Observation in the Gas Phase in 1976
- Ethenol appeared in no Flame Chemistry Model

Reaction of C_2H_4 with OH is One Possible Mechanism to Form Ethenol

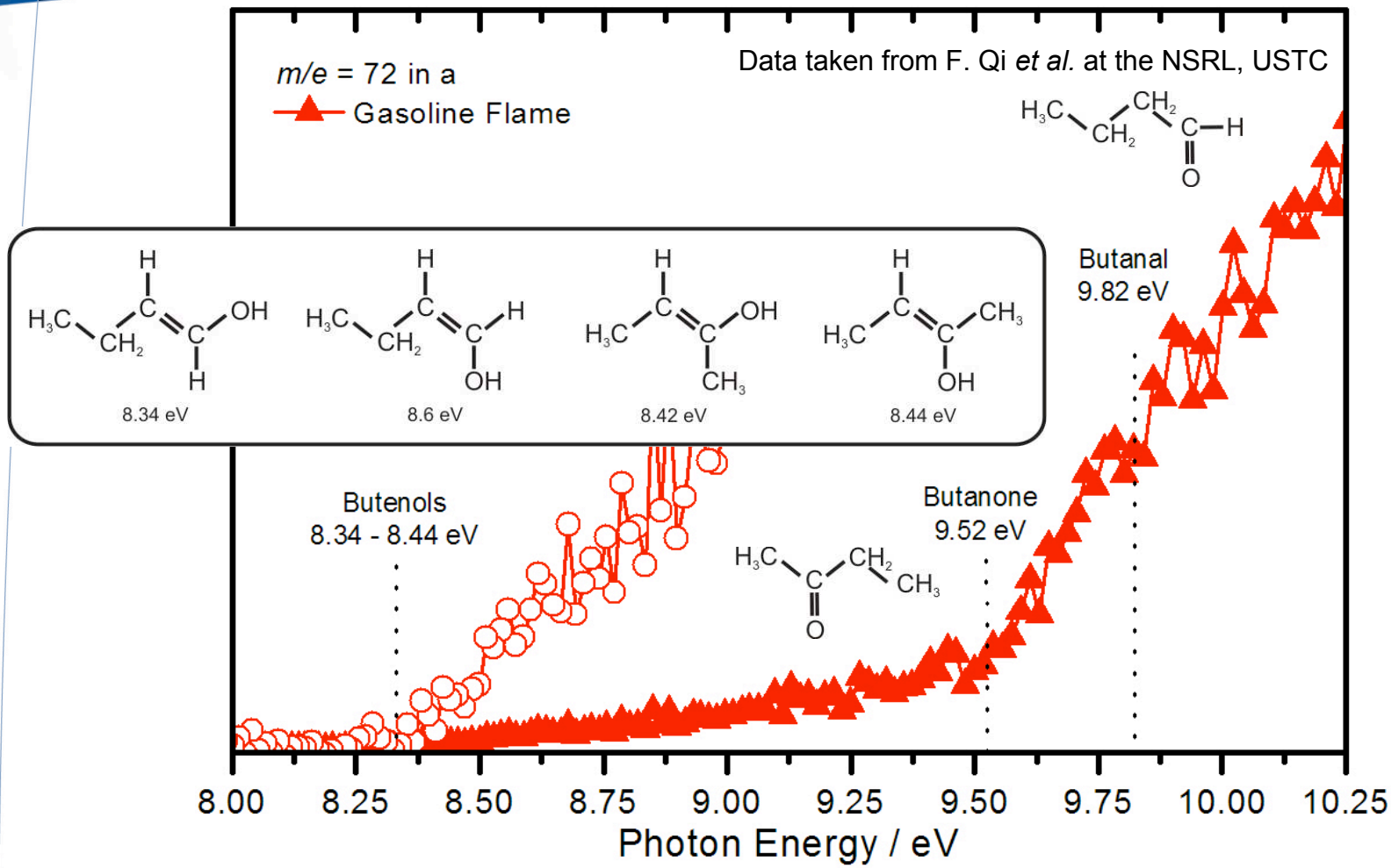


- ✓ Is Dehydrogenation of alcohols a possible route to Enols?
- ✓ Are higher enols (Propenol, Butenol ...) important?

Enols are Common Combustion Intermediates – Detection of Propenols



Enols are Common Combustion Intermediates – Detection of Butenols



Achievements and Conclusions

- ✓ More than 25 different flames have been characterized:
  - ➢ methane, ethane, propane, ethene, propene, allene, butadiene, acetylene, propyne, cyclopentene, cyclohexane, benzene, ethanol, isopropanol, n-propanol, dimethylether, methylacetate, ethylformiate
- ✓ Online database is currently under construction

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Summary and Conclusions:

- ✓ Molecular Beam-Mass Spectrometry with synchrotron VUV photoionization is a powerful new tool
- ✓ Even after 150 years of research there are still new things in flames to discover
- ✓ Enols are common combustion intermediates

Acknowledgements

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