

MeV-UED Run-4 Summary and Future Capabilities on Chemical Science

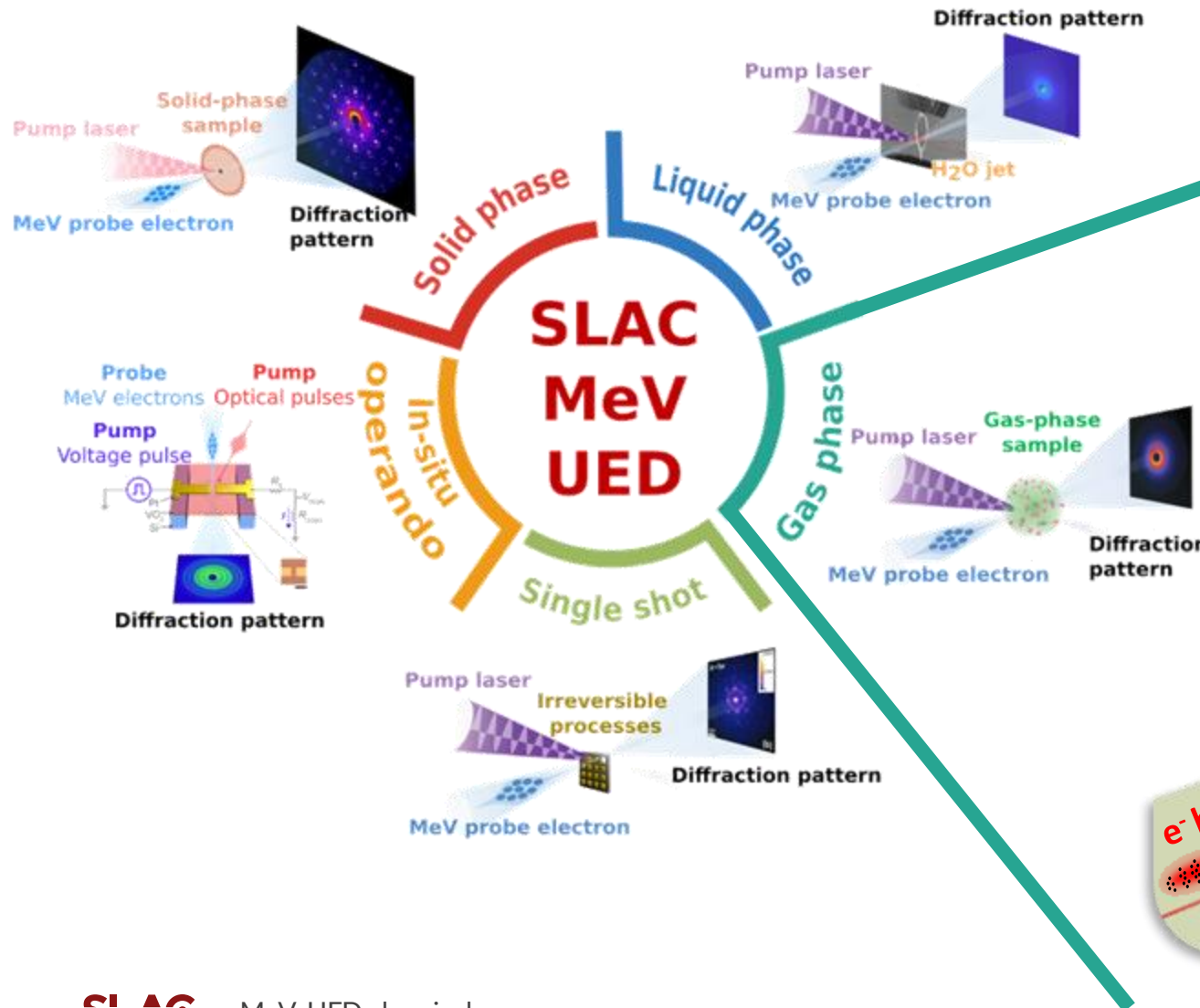
MeV-UED Instrument Advisory

MeV-UED, AD, LCLS

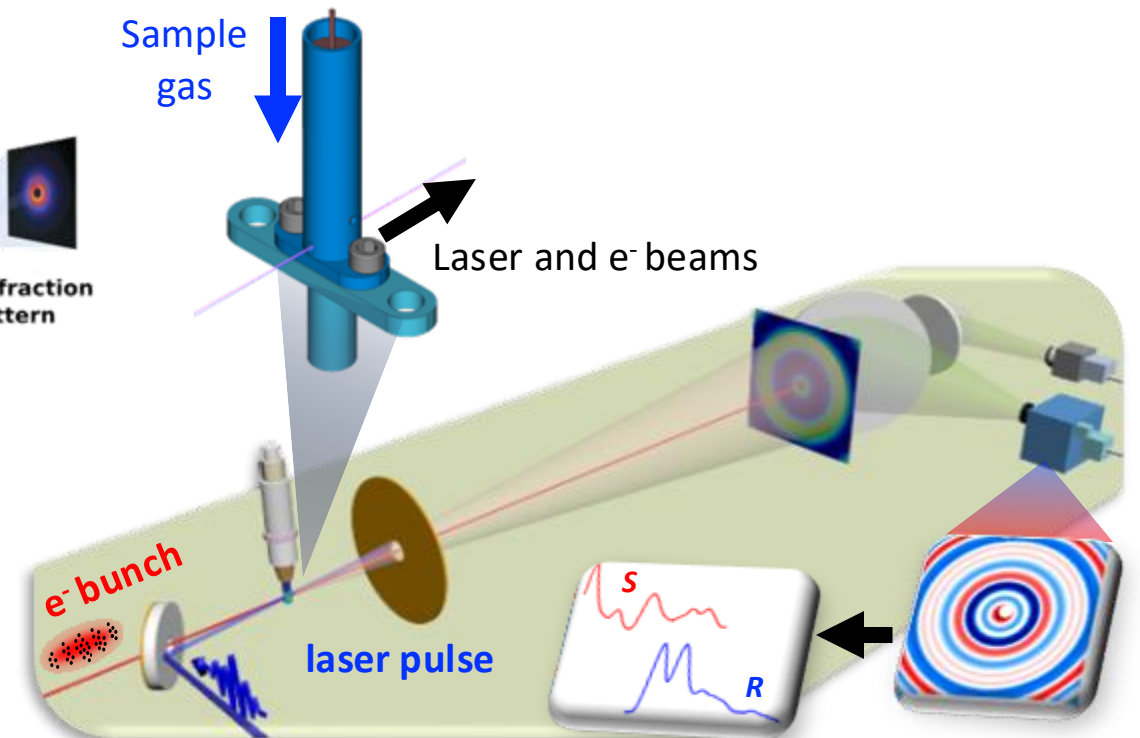
Nov. 18th, 2024

Yusong Liu

Gas-Phase Chemical Science Program in MeV-UED

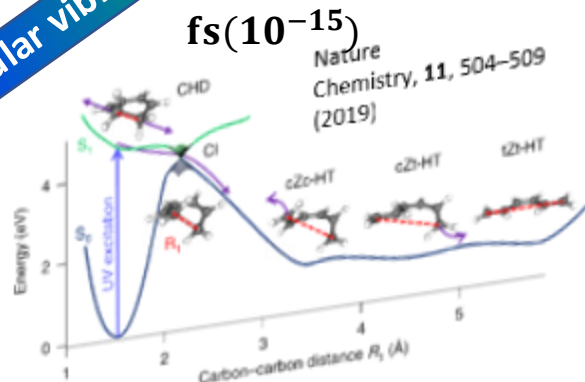
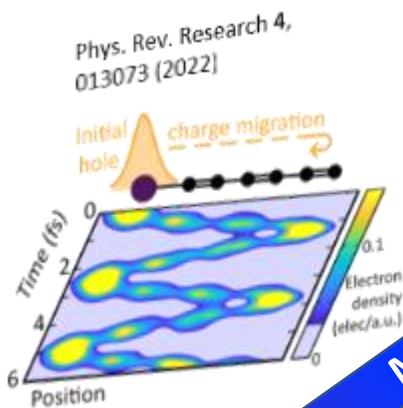
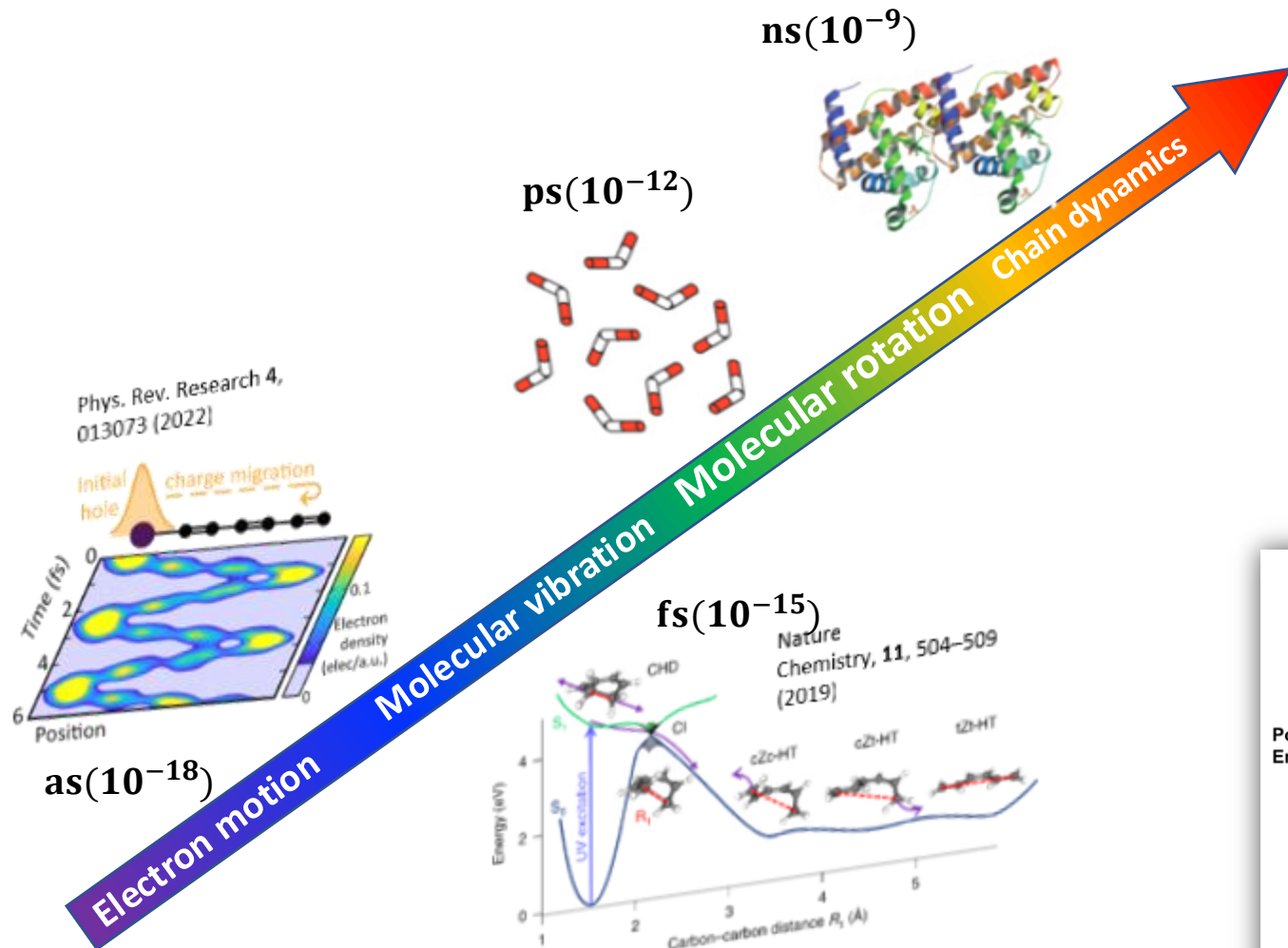


Electron energy (E_{ke}): 3.7 MeV
 Temporal resolution: 150 fs
 Q range: 1-10 Å⁻¹
 Spatial resolution: <0.6 Å

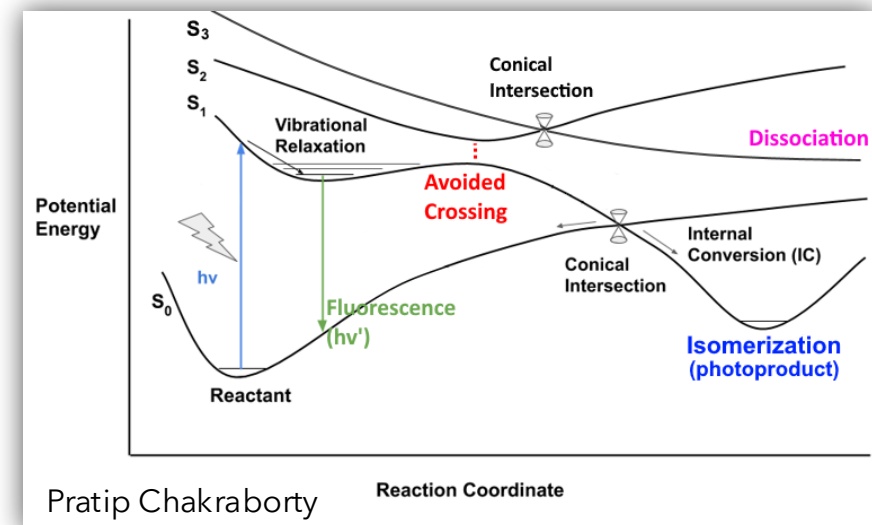
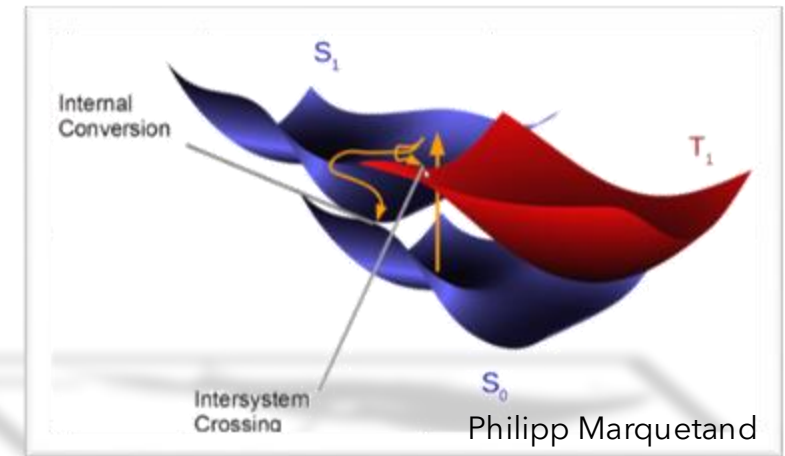


Gas-Phase Chemical Science Program in MeV-UED

Molecular excited state dynamics and photochemistry

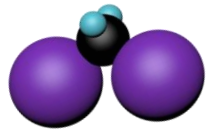


Coupled electron-nuclear dynamics

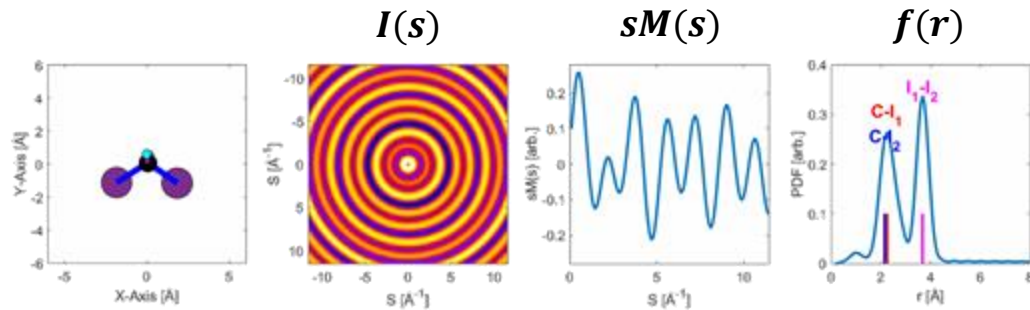


Gas-Phase Chemical Science Program in MeV-UED

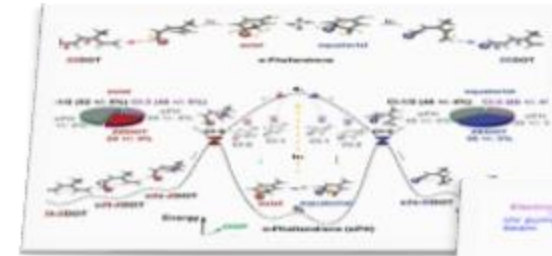
Direct structural probe within femtosecond temporal resolution



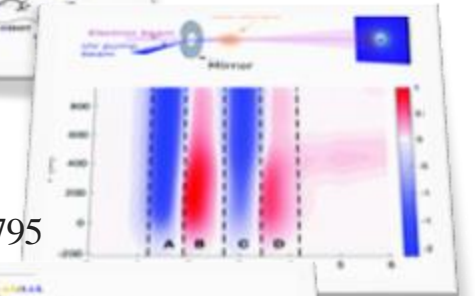
$C-I_1, C-I_2, I_1-I_2, \dots$



Science, 2021, 374, 6564, 178-182



PCCP, 2022, 24, 15416-15427



Nat Commun 14, 2795 (2023)

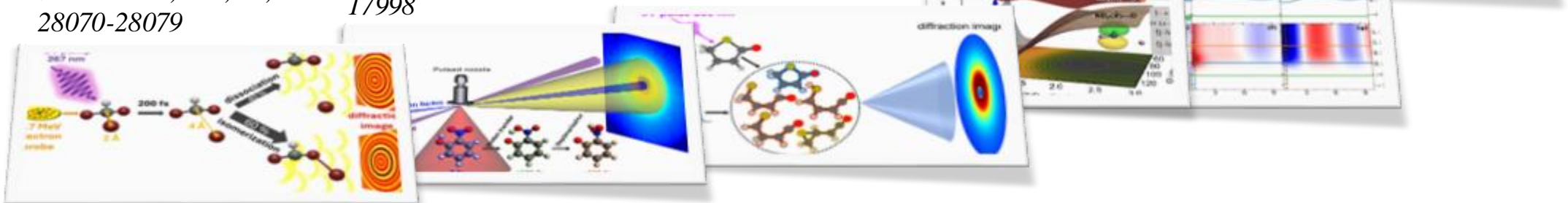
From **Diffraction pattern** to **pair distribution function (PDF)**

PRL. 131, 143001 (2023)

JACS. 2024, 146, 41, 28070-28079

PCCP, 2024, 26, 17991-17998

JACS. 2024, 146, 6, 4134-4143

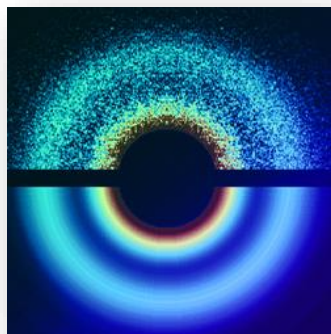


Gas-Phase Chemical Science Program in MeV-UED

Theoretical verification from UED measurement observables



JOURNALS > UPCOMING SPECIAL TOPICS > THE JOURNAL OF CHEMICAL PHYSICS >
PREDICTION CHALLENGE: CYCLOBUTANONE PHOTOCHEMISTRY

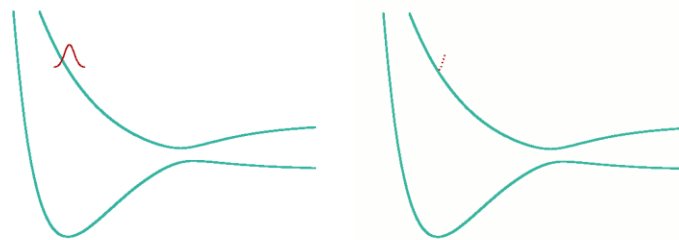


Prediction Challenge:
Cyclobutanone Photochemistry

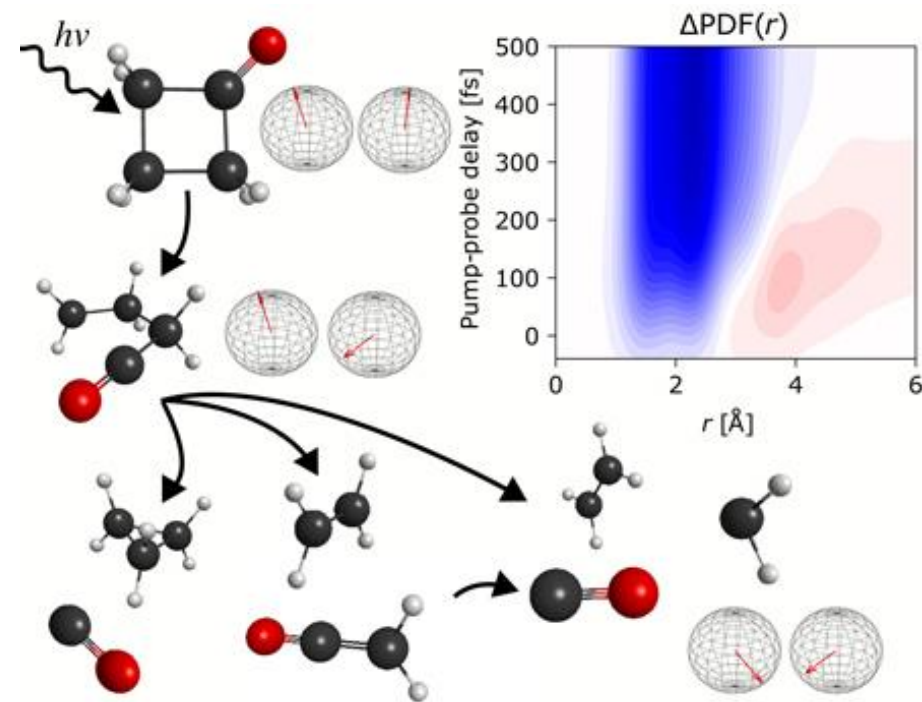
15 manuscripts were submitted

Submission Deadline: February 15, 2024

Todd Martínez



Dr. Marianna Assmann



Experiment: Run-4, UED119, Jan. 21st, 2024

Alice Green Thomas Wolf



Experiments summary and capabilities development

Discussion agenda

- ❖ Gas Phase Chemical Program in SLAC MeV-UED
- ❖ **Run-4 gas phase UED experiment summary**
 - Run-4 experiments and operation
 - Newly emerged experimental capabilities
- ❖ **GUED ongoing R&D efforts towards to future experimental capabilities**
 - Deep UV light generation
 - Slit-jet sample delivery
 - Electron detection and diagnostics
- ❖ **Conclusion**

Summary of Run-4 GUED experiments

GUED Run-4, Nov. 2023 to Jun. 2024

- ❖ Very successful user run
 - Many experiments accomplished
 - Two sample delivery protocols offered
 - Multiple laser excitation wavelengths

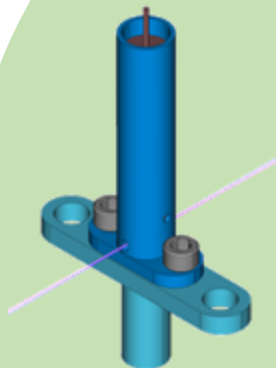
**Laser
wavelengths**

266 nm

OPA(245, 300, 330 nm)

200 nm

Flow-cell



U122 Ramasesha

U120 Liu

U101 Centurion

U108 Forbes

U110 Suits-Rolles

U114 Ihee

U113 Yang

U119 Green

U100 Weber

U116 Minns

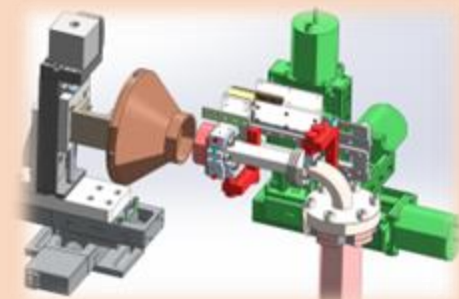
U112 Allum

U115 Gühr

U102 Wolf

U113 Cheng
(200, 266 nm)

U124 Lin
(266, 300, 330 nm)

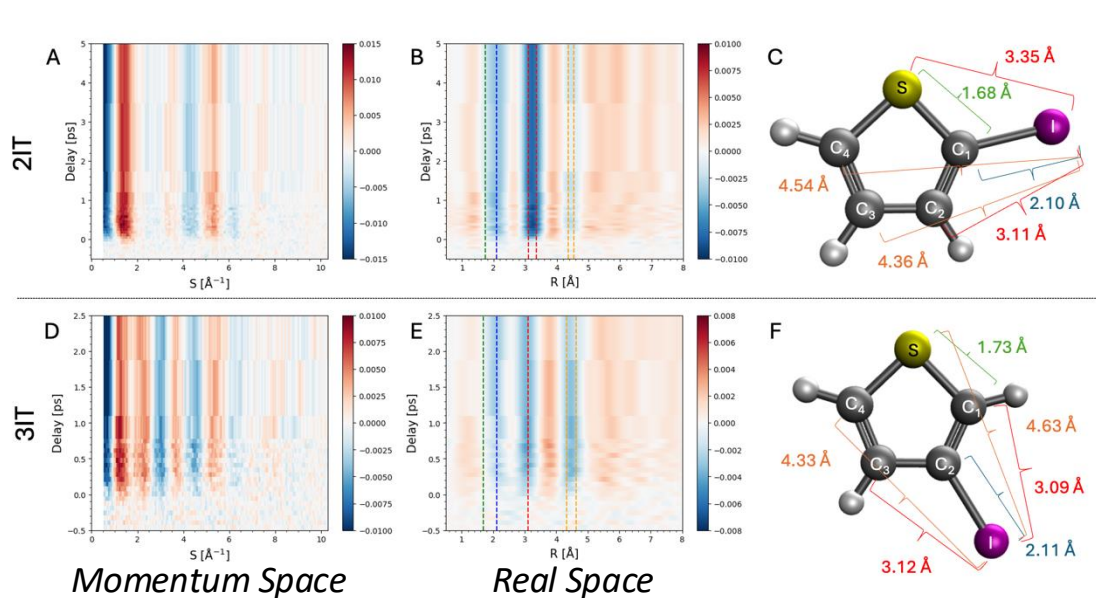


Slit-Jet

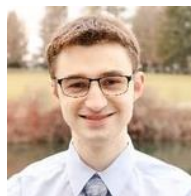
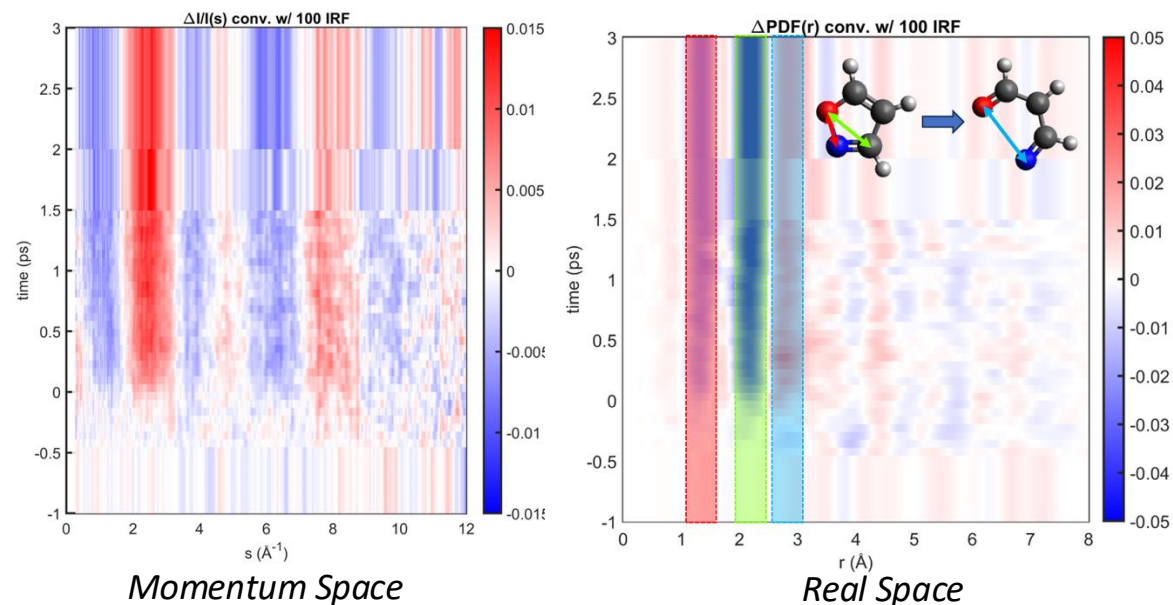
Summary of past Run-4 GUED experiments operation

Beamtime highlights

Direct vs. Stepwise iodine elimination in 2- and 3-Iodothiophenes



Ring-opening and isomerization of Oxazole



Aaron Ghrist



Matthew Bain



Ruaridh Forbes

U108 Forbes

U110 Suits-Rolles



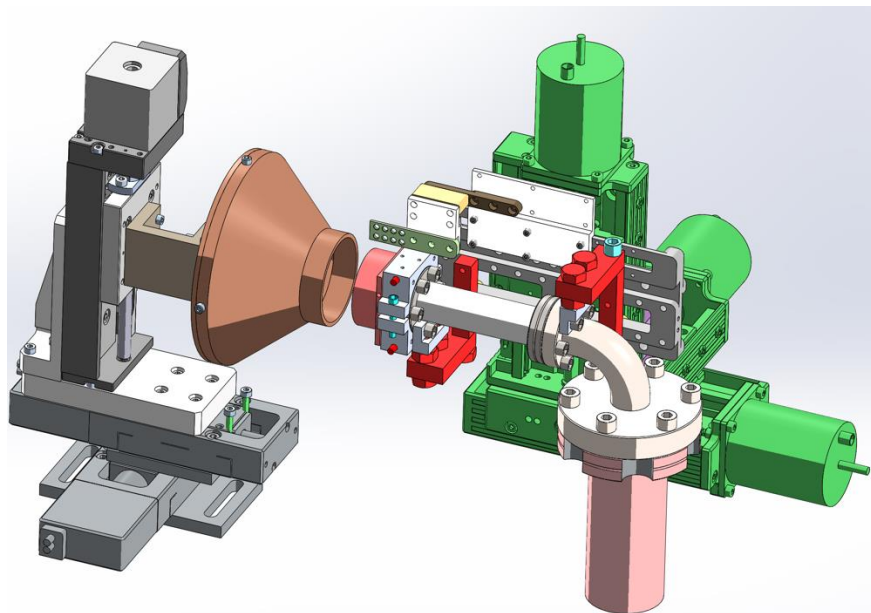
Huynh Lam



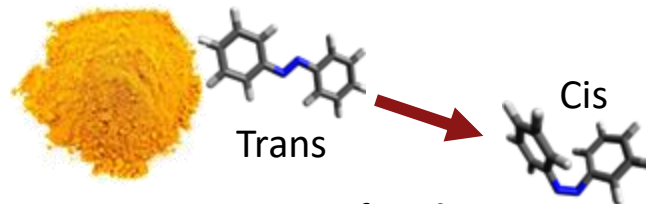
Daniel Rolles

Summary of Run-4 GUED experiments operation

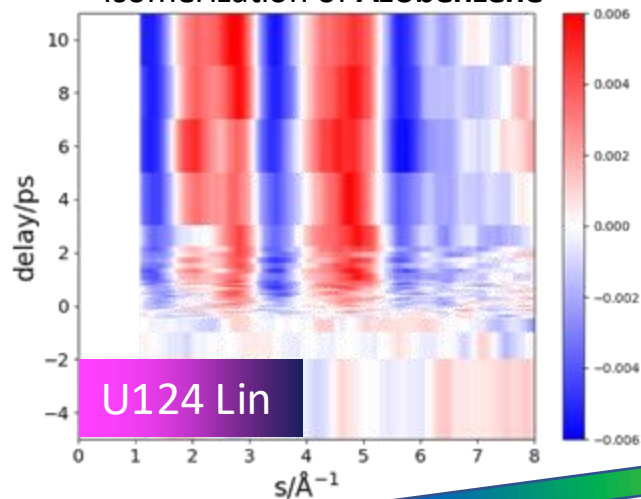
Slit-Jet sample delivery low-vapor pressure samples



Sample delivery above ambient temperature
50-500 °C
Led by Ming-Fu Lin



Isomerization of Azobenzene



Delivery at 120 °C

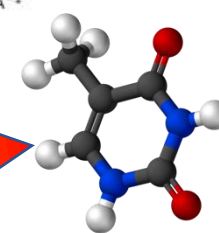
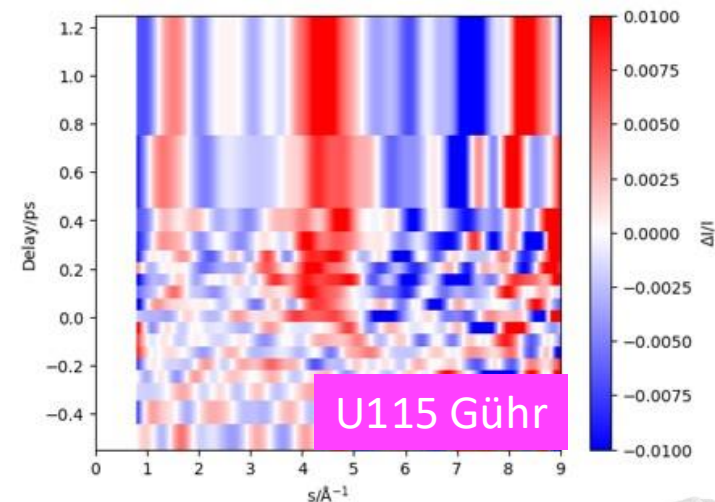


Surjendu Bhattacharyya

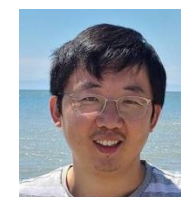


Ming-Fu Lin

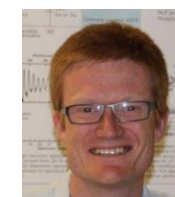
Relaxation of Thymine



Delivery at 250 °C



Xiaojun Wang



Markus Gühr

Summary of Run-4 GUED experiments operation

Take home messages

Achievements

- ❖ Standard configuration with **flow-cell**
 - Stable running condition with efficient usage of machine hours
 - Consistently high success rate with the refined capabilities
- ❖ New capabilities expanding science cases with **slit-jet sample delivery**
 - Successful transition from R&D to user experiments
 - Running up to 250 °C for a Torr level.
 - High quality data for user experiments
- ❖ MeV-UED user community expended in chemical science

Remining challenging need further efforts

- ❖ Higher repetition rate (Joel's talk),
 - ❖ Pushing from 360 Hz to 1080 Hz
- ❖ Higher sensitivity in electron detections
 - ❖ Andor optical camera
 - ❖ ePix direct detector
- ❖ Further improvement on the sample delivery
 - ❖ Slit-jet sample delivery
 - ❖ Up to 500 °C.
- ❖ Strong need for improvement of temporal resolution

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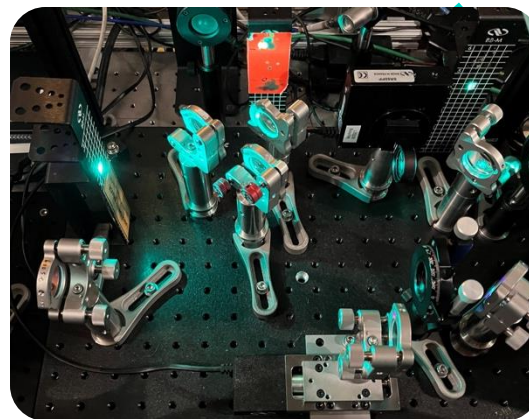
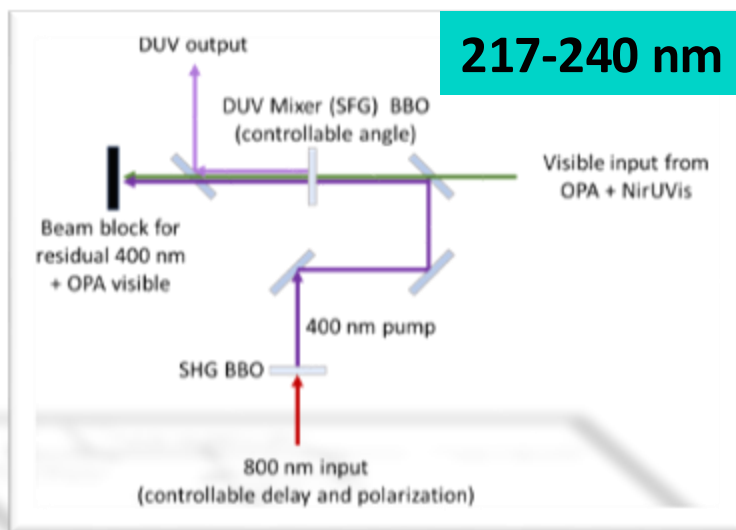
Ongoing R&D efforts enabling new capability in GUED

Improvement in laser capabilities

Current laser capabilities in MeV-UED

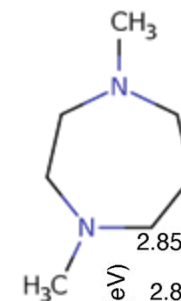
200 nm, 240 nm – 2.4 μm , mid-IR up to 12 μm , THz (100 - 300 μm)

Gap between 200 and 240 nm (Deep UV generation)

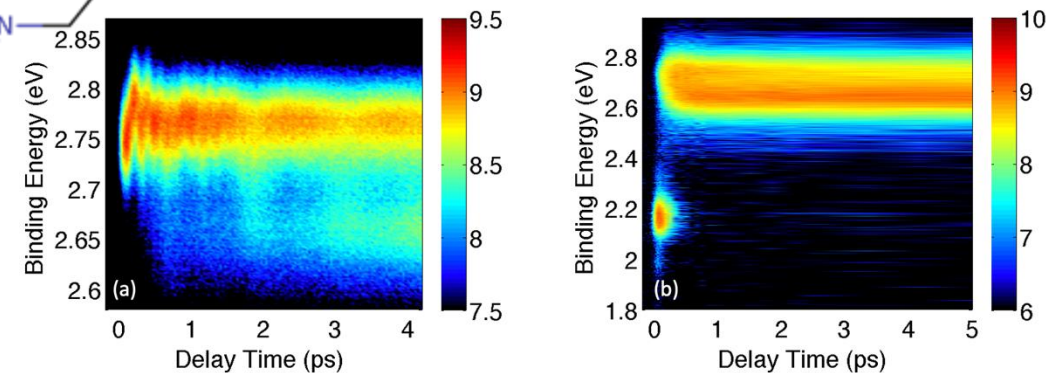


10s of μ

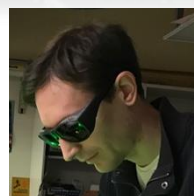
Photo-relaxation dynamics of DMHP at DUV regime



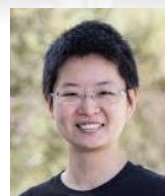
1,4-dimethyl-1,4-diazepane (DMHP)



Photoelectron spectra of DMHP excitation at 238 nm and 205 nm (provided by *Xinxin Cheng*)



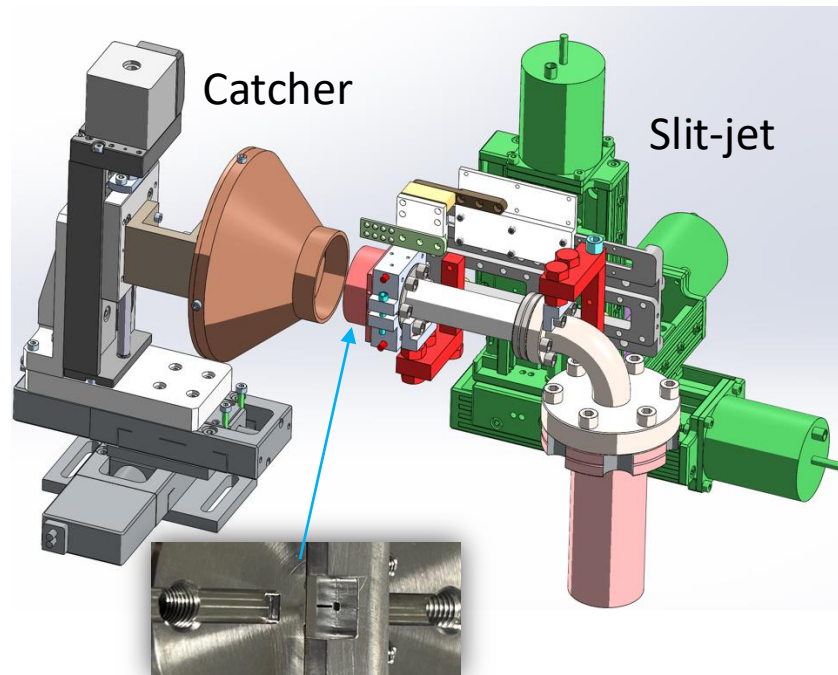
Patrick Kramer



Xinxin Cheng

Ongoing R&D efforts enabling new capability in GUED

Improvement in sample delivery system



❖ Slit-jet (Ming-Fu Lin and team)

- Motion and alignment control
- Keep optimizing the designing
- Active cooling (operation efficiency)

❖ Catcher

- Dynamic monitoring of sample accumulation
- Larger capacity of sample
- Optimizing the structure

❖ Further testing

- Pushing towards to 500 °C



Ongoing R&D efforts enabling new capability in GUED

Improving electron detection and characterization

❖ Andor optical camera and ePix10K electron direct detector

➤ Andor optical imaging system (phosphor to EMCCD)

- Larger Q range, higher collection efficiency, Less imaging distortion

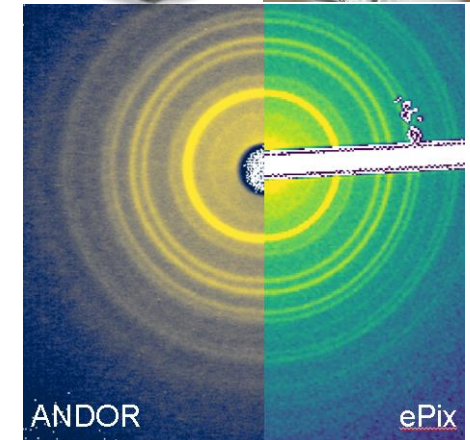
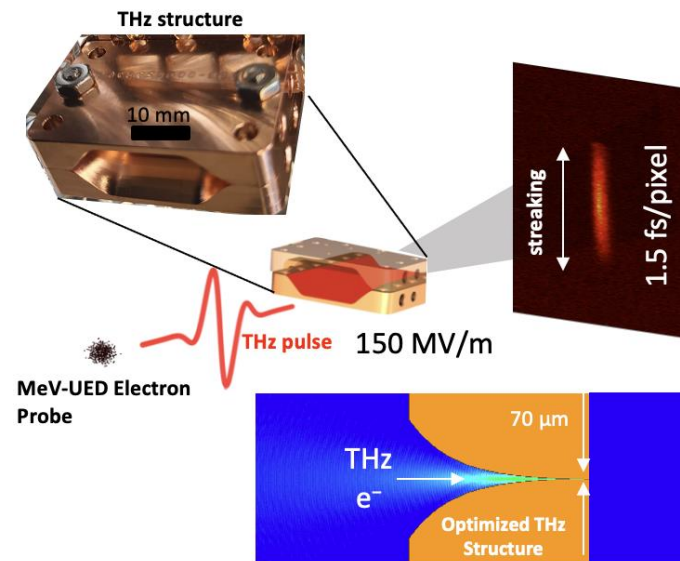
➤ ePix direct detector

- Higher detection sensitivity, larger Q range, Single-shot detection

❖ Improvement on temporal resolution (THz-based streaking time-tool)

➤ Push from 150 fs to sub-100 fs or even shorter

➤ Feasible to observe fast wavepacket dynamics and structure changes



Diffraction patterns
Andor vs. ePix

shot-to-shot
Jitter and duration.

Conclusion

❖ Run-4

Significant achievements and insights into ultrafast chemical dynamics enhancing our understanding of rapid molecular transformations.

❖ Ongoing R&D efforts

Through continuous efforts in R&D projects, we have established various *new capabilities*, including advanced sample delivery methods, expanded laser wavelength options, enhanced electron detection techniques, and pushing to the improvement of temporal resolution.

❖ Looking forward

Continued advancements in high performance of the electron source and detector technology will further enhance MeV-UED's precision, opening new pathways for studying complex reactions and dynamic processes central to chemical innovation.

Acknowledgements

MeV-UED team members



Alex Reid



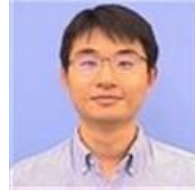
Mike Minitti



Joel England



Xiaozhe Shen



Fuhao Ji



Stephen Weathersby



Cameron Duncan



Tianzhe Xu



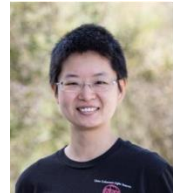
Sharon Philip



Thomas Wolf



Ming-Fu Lin



Xinxin Chen



Yusong Liu



Surjendu Bhattacharyya



Jake Koralek



Mianzhen Mo



Stanford
University



Patrick Kramer



Matthias Hoffmann



Brian Kaufman



Randy Lemons



Samul Eisenberg



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ENERGY