Oregon State University

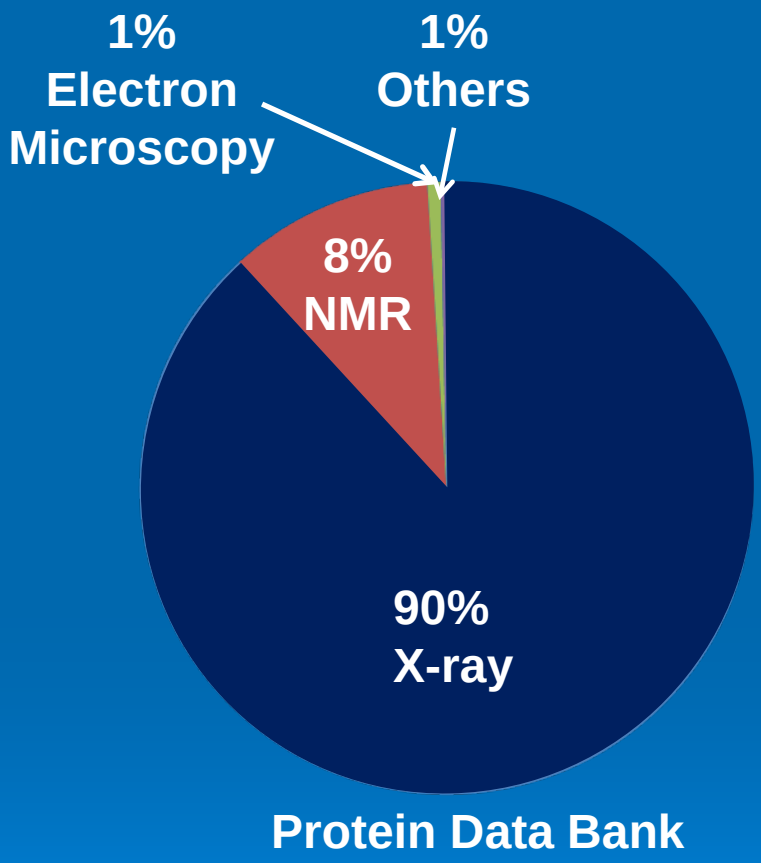
Wei Kong, Chemistry

Serial single molecule electron diffraction imaging: A Journey

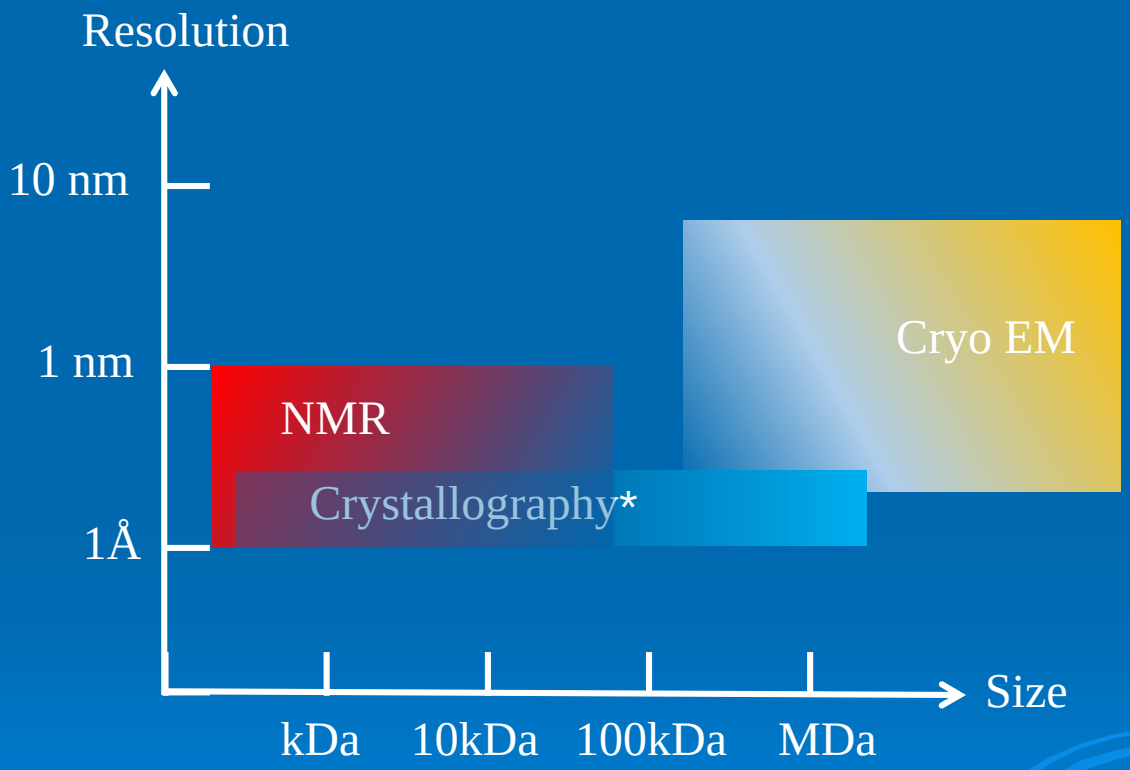
Outline

- Serial single molecule electron diffraction imaging
- Results
  - Electron diffraction of neutral molecules in droplets
  - Doping proteins – GFP
- Unique properties of large droplets
- The journey continues …

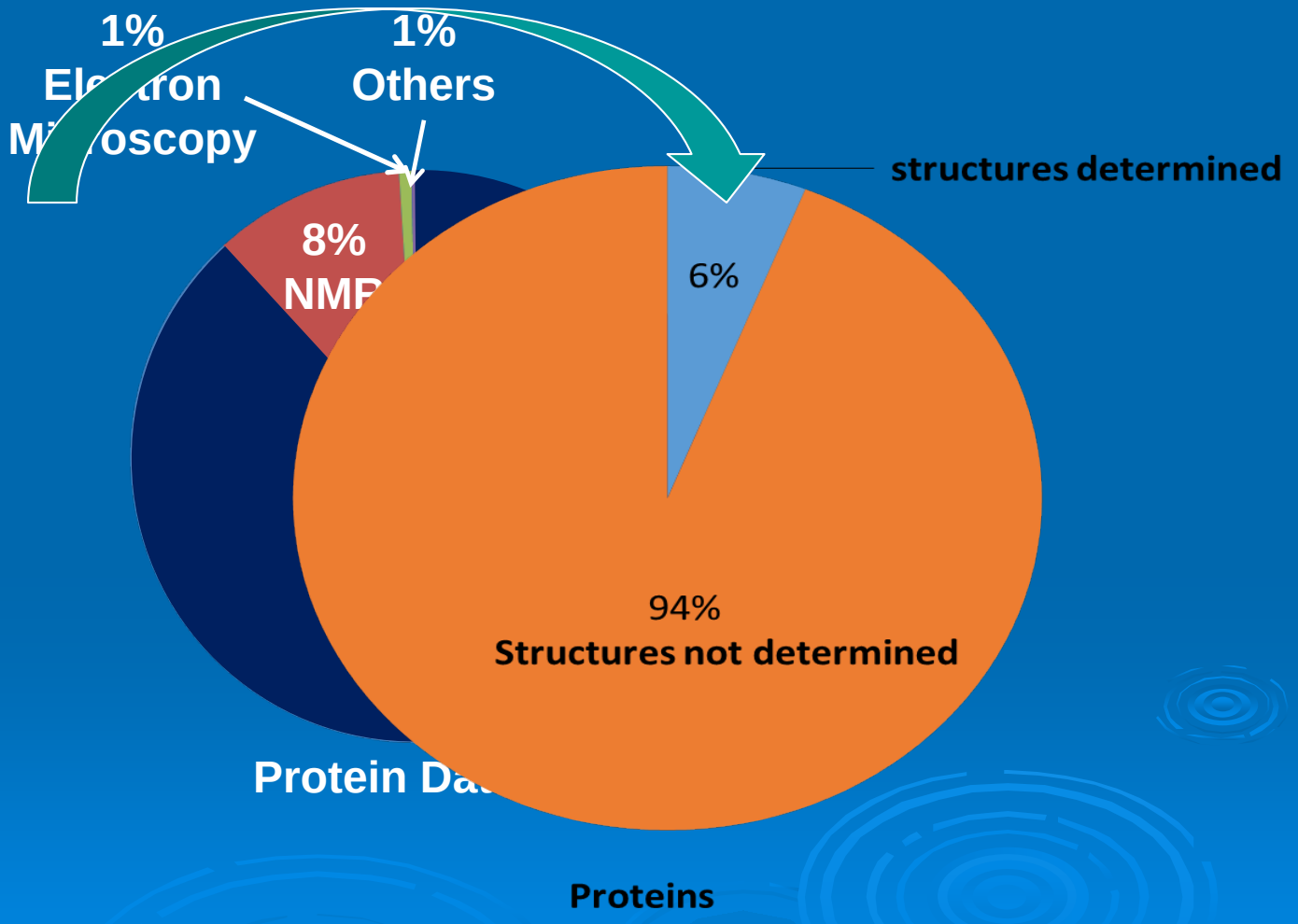
Structure Tools Comparison



Structure Tools Comparison



State of the Field



Single Molecule Diffraction

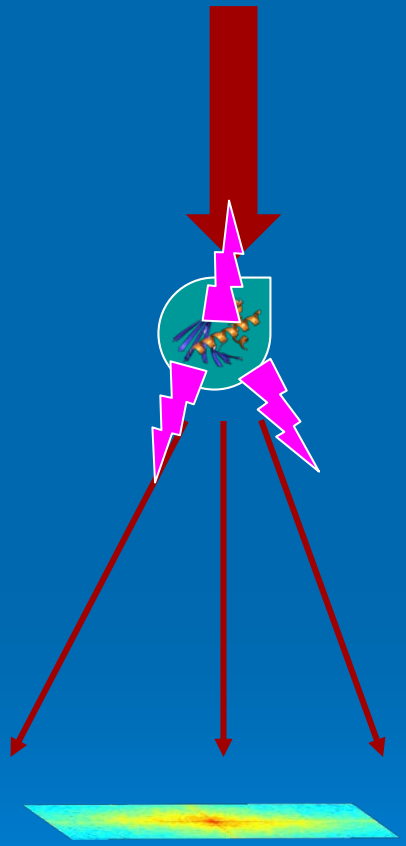
- ✓ “Diffract & Destroy”

  Neutze, R., Wouts, R., van der Spoel, D., Weckert, E. and Hajdu, J., Nature 406 (2000) 752.

- ✓ Serial Single molecule Electron Diffraction Imaging (SS-EDI)

  Beckmann, Kong, Voinov, Freund, US Patent: 9,279,778 (2016).

Diffract & Destroy



Diffract & Destroy

- Each particle produces one image
- Each image may be from a different orientation
- Particle orientation needs to be determined from image
- Orientational distribution has to be uniform

Diffract & Destroy

- Light source: intense & short (< 100 fs)
- Detector: high quality
- Image: good enough for orientation assignment

Diffract and Destroy

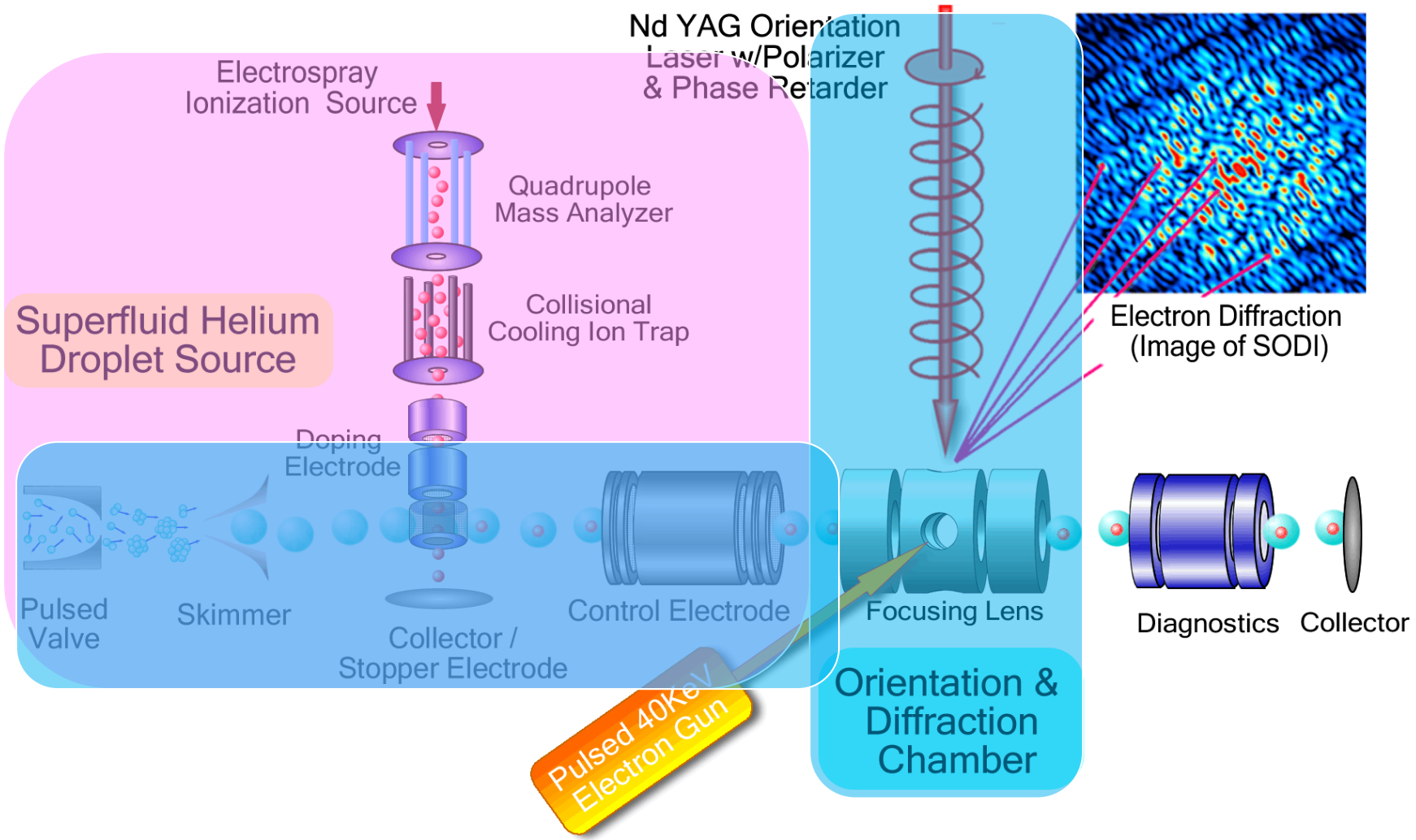
Diffract & Destroy

- Electrons vs nuclei?
- Electron movement: < 1 fs

IMPOSSIBLE?

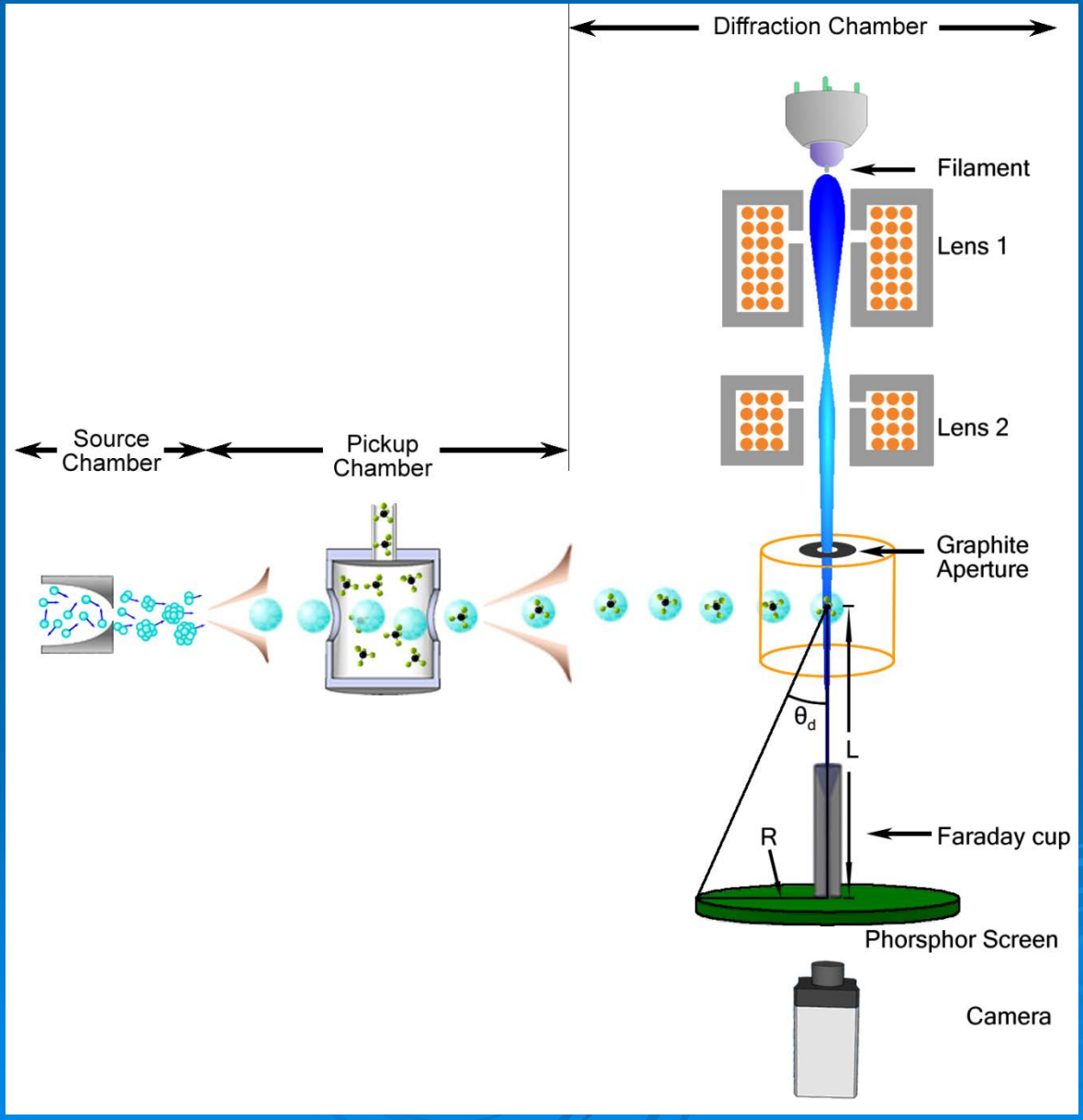
Fratalocchi, A. and Ruocco, G., "Single-molecule imaging with X-ray free-electron lasers: Dream or reality?" Phys. Rev. Lett. 106 (2011) 105504.

Serial Single molecule Electron Diffraction Imaging (SS-EDI)



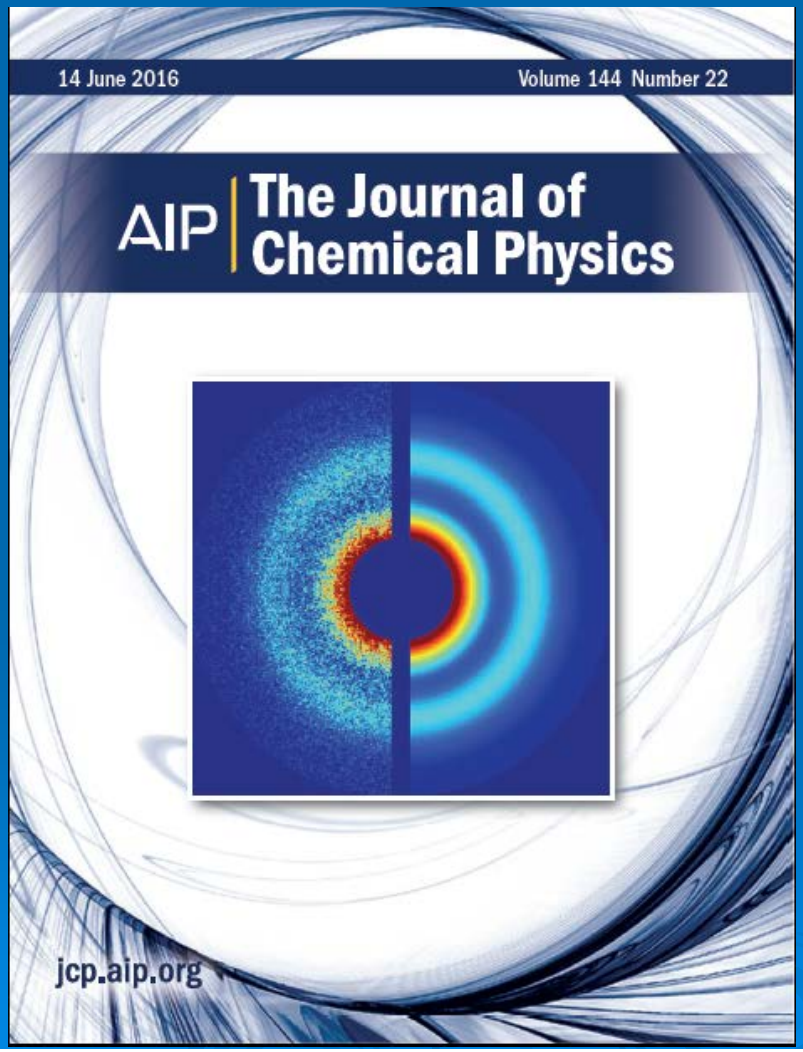
Beckmann, Kong, Voinov, Freund, US Patent: 9,279,778

Diffraction Half



Diffraction Half

Electron diffraction of ferrocene in droplets



Zhang, He, and Kong, J. Chem. Phys. **144**, 221101 (2016).

Diffraction Half

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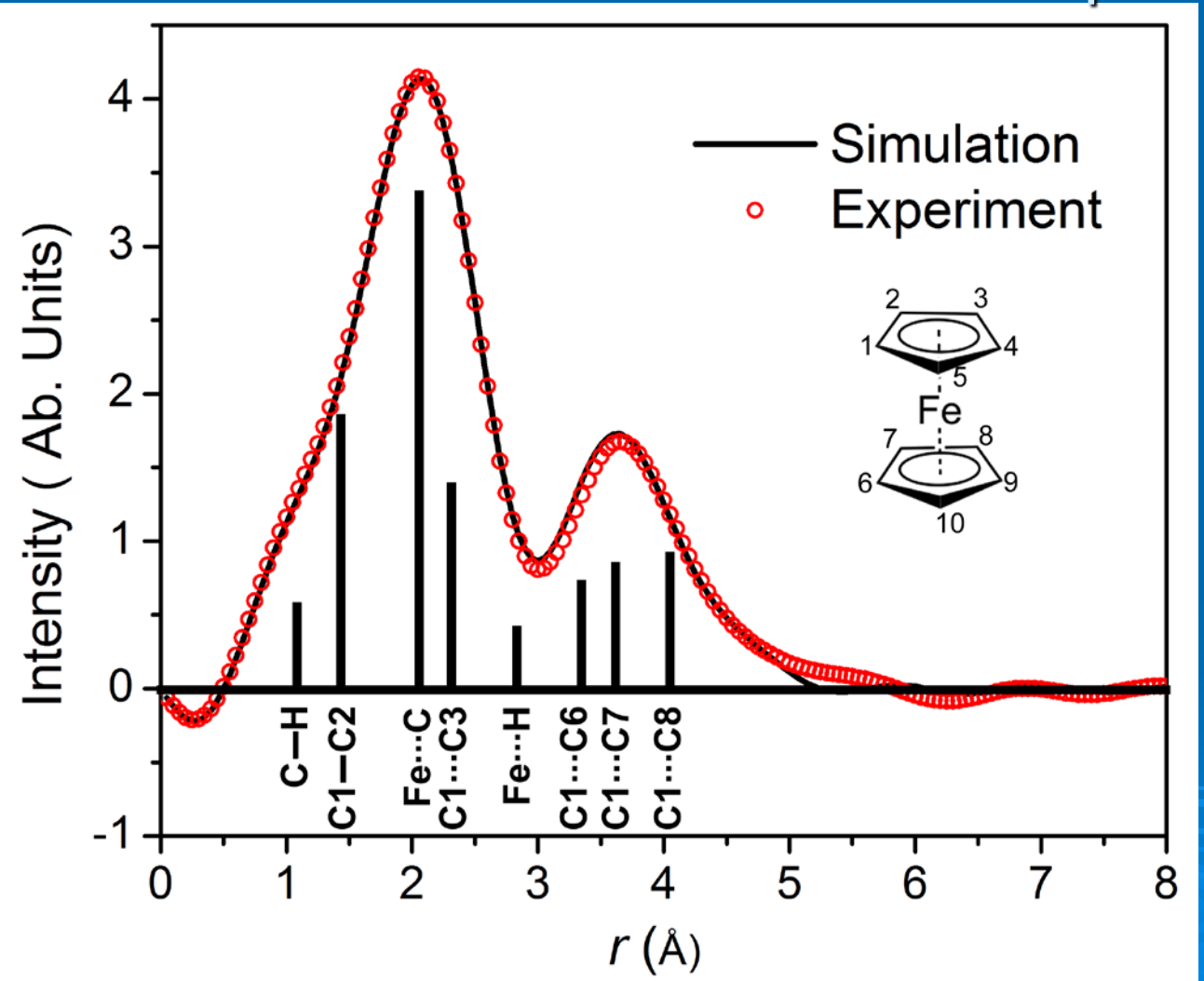
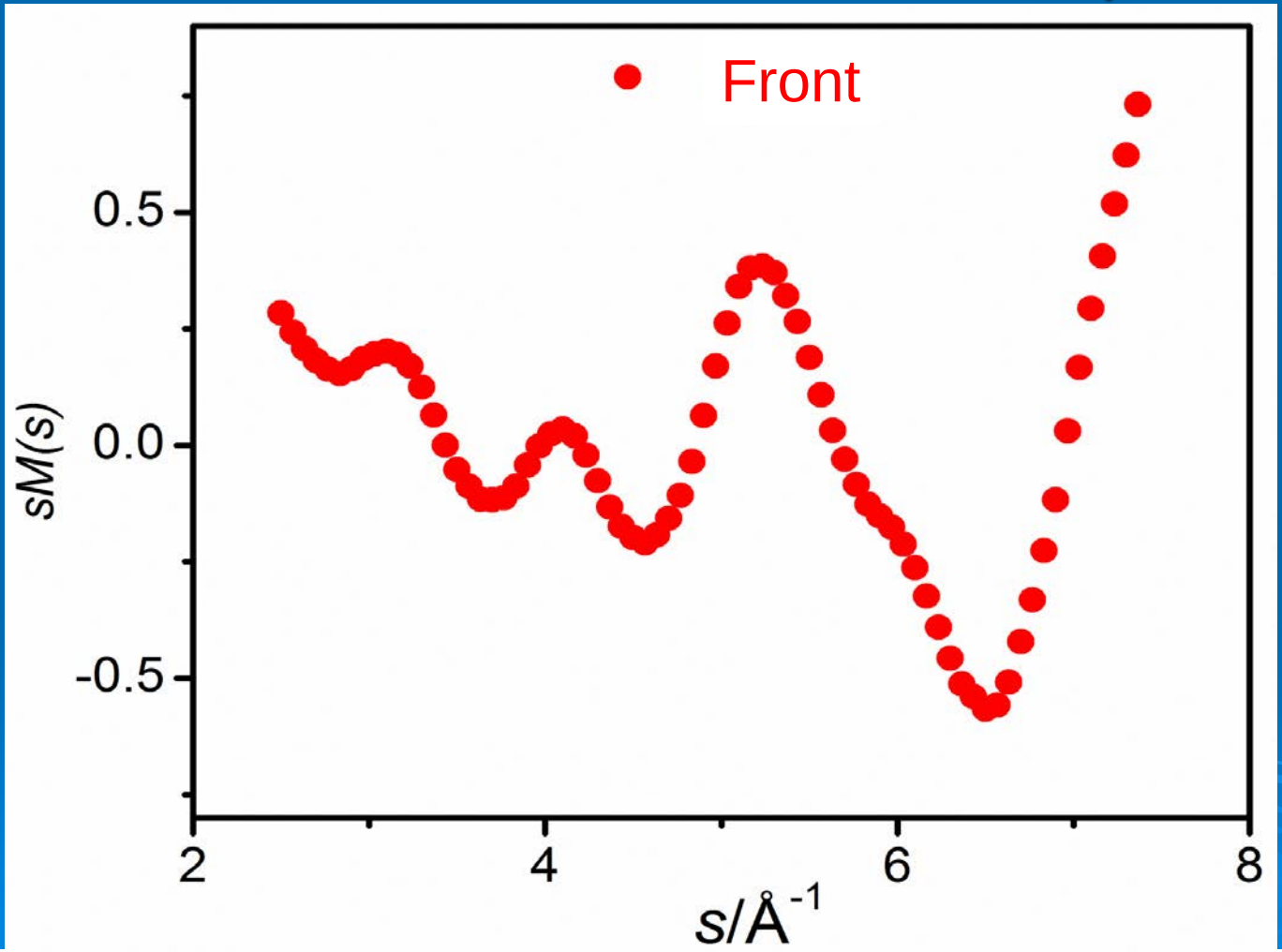


Zhang, He, and Kong, J. Chem. Phys. **144**, 221101 (2016).

Diffraction Half

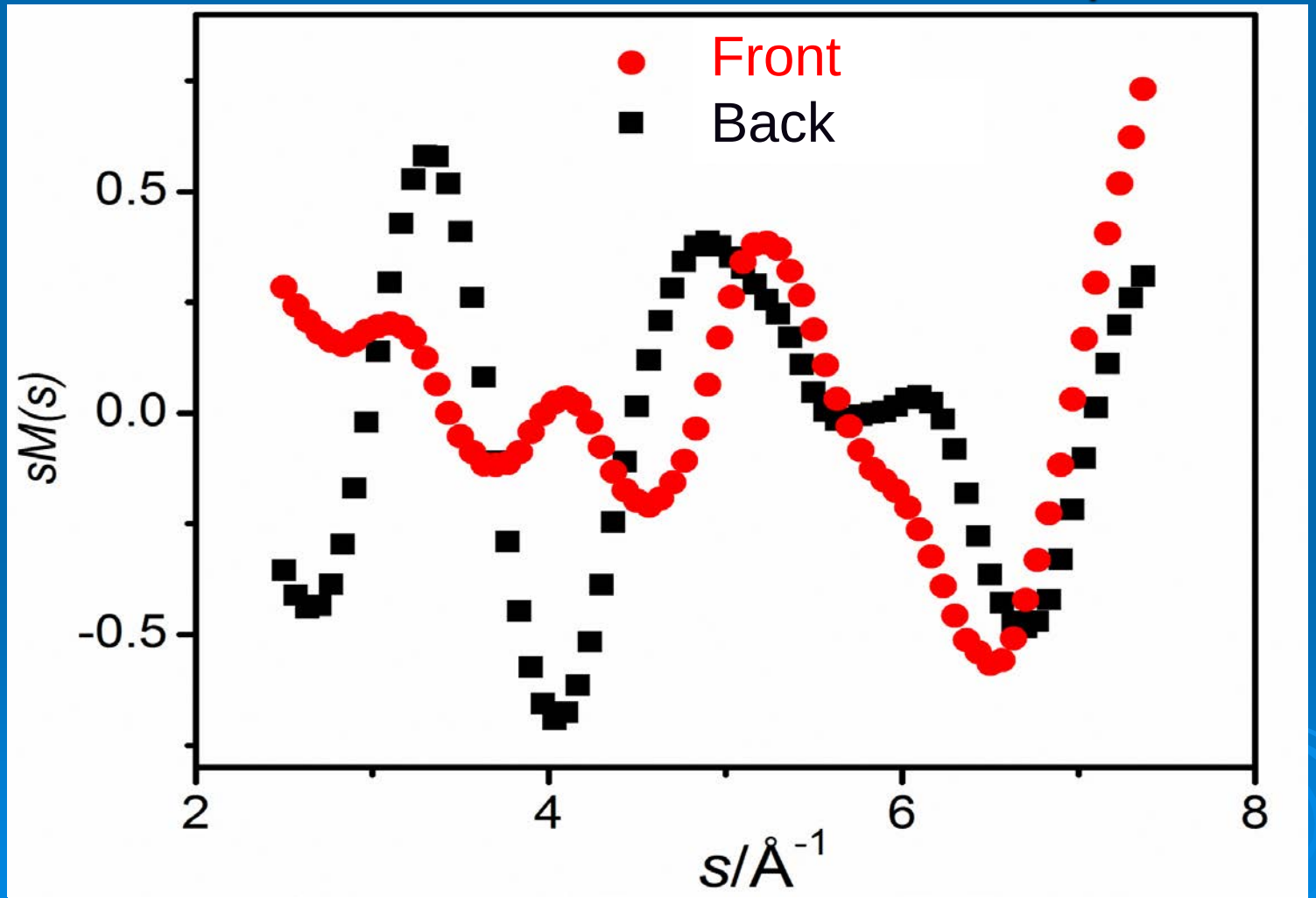
Electron diffraction of Iodine in droplets



He, Zhang, Lei, and Kong, Angew. Chem. Int. Ed. **56**, 3541 (2017)

Diffraction Half

Electron diffraction of iodine in droplets



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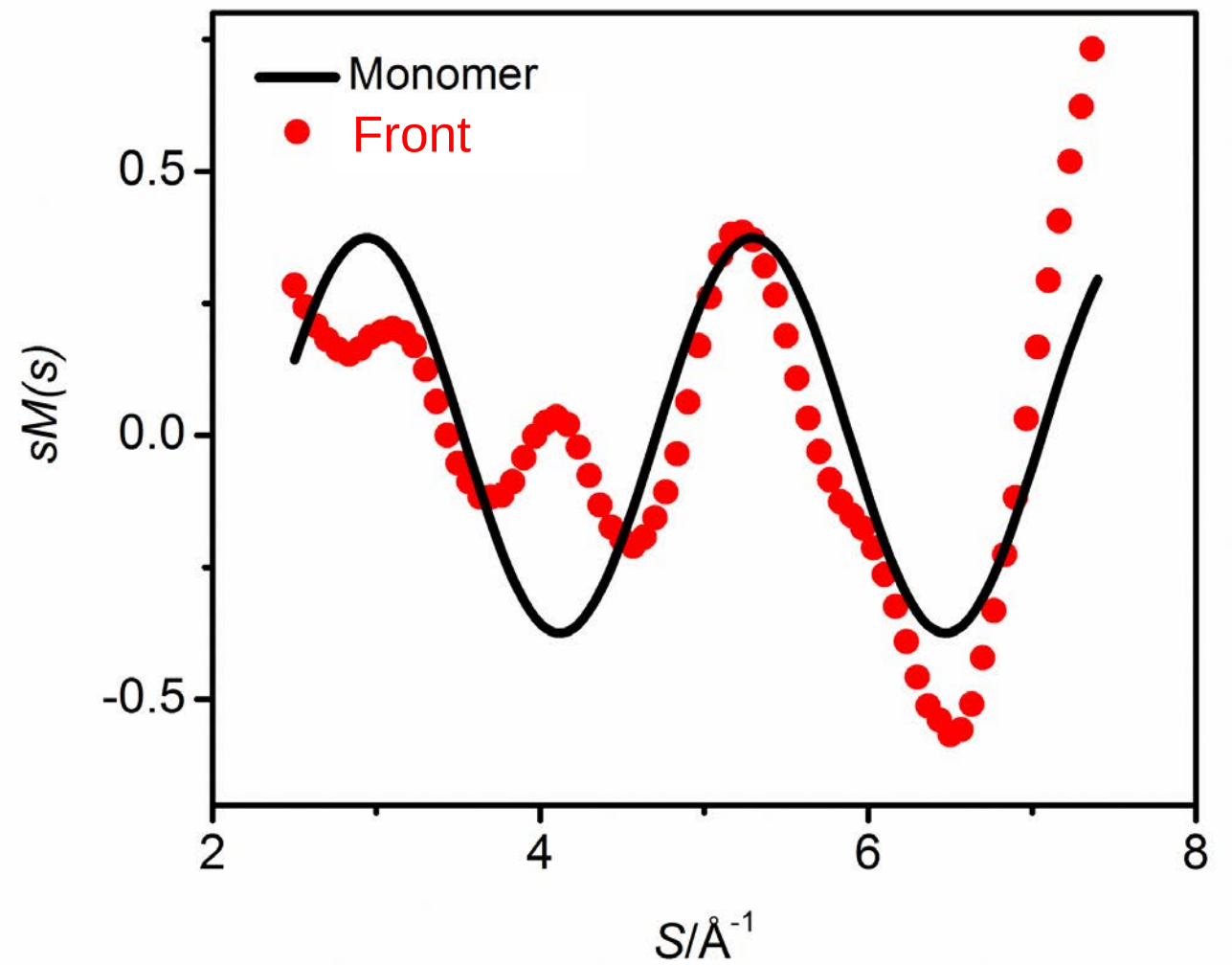

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Diffraction Half

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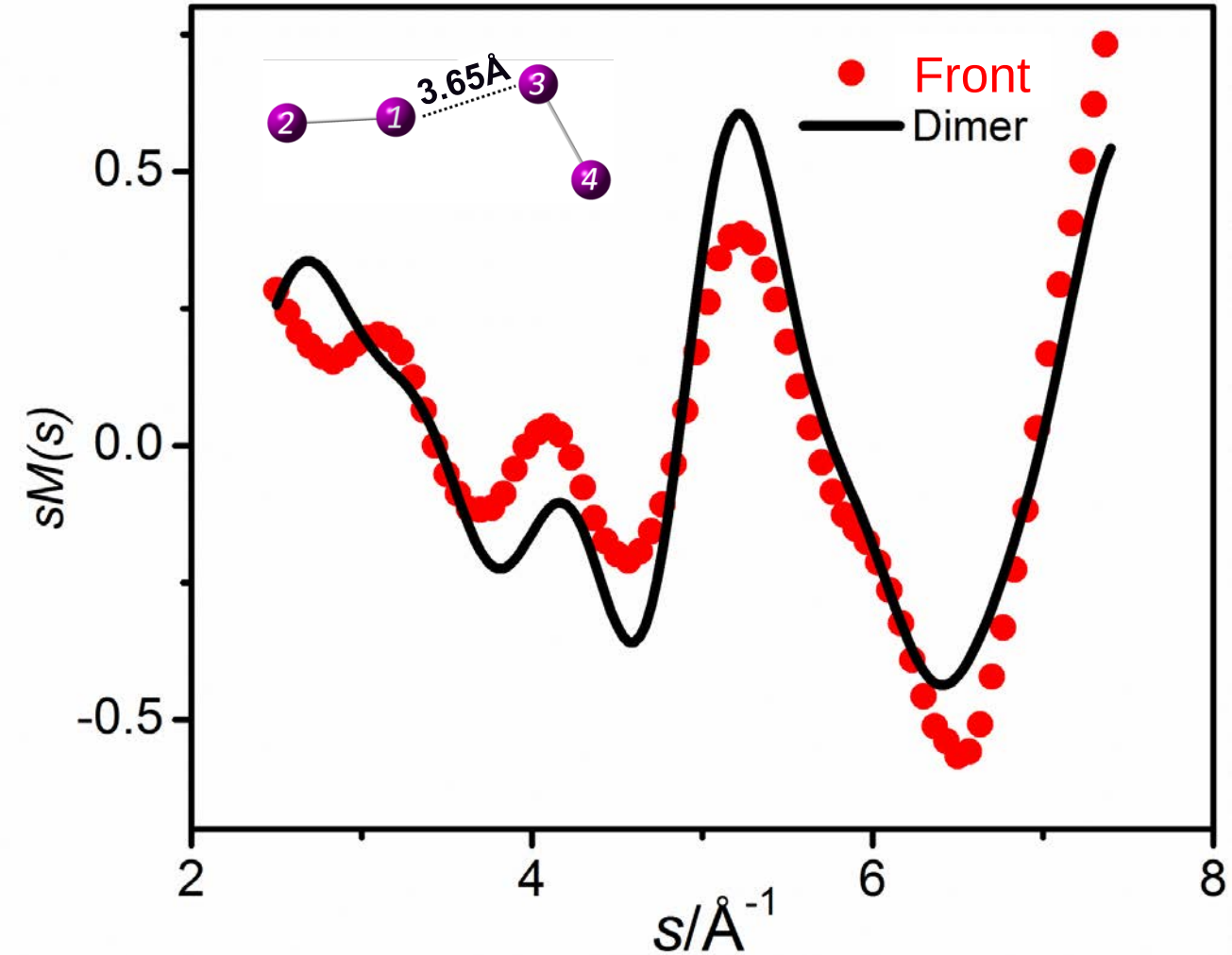
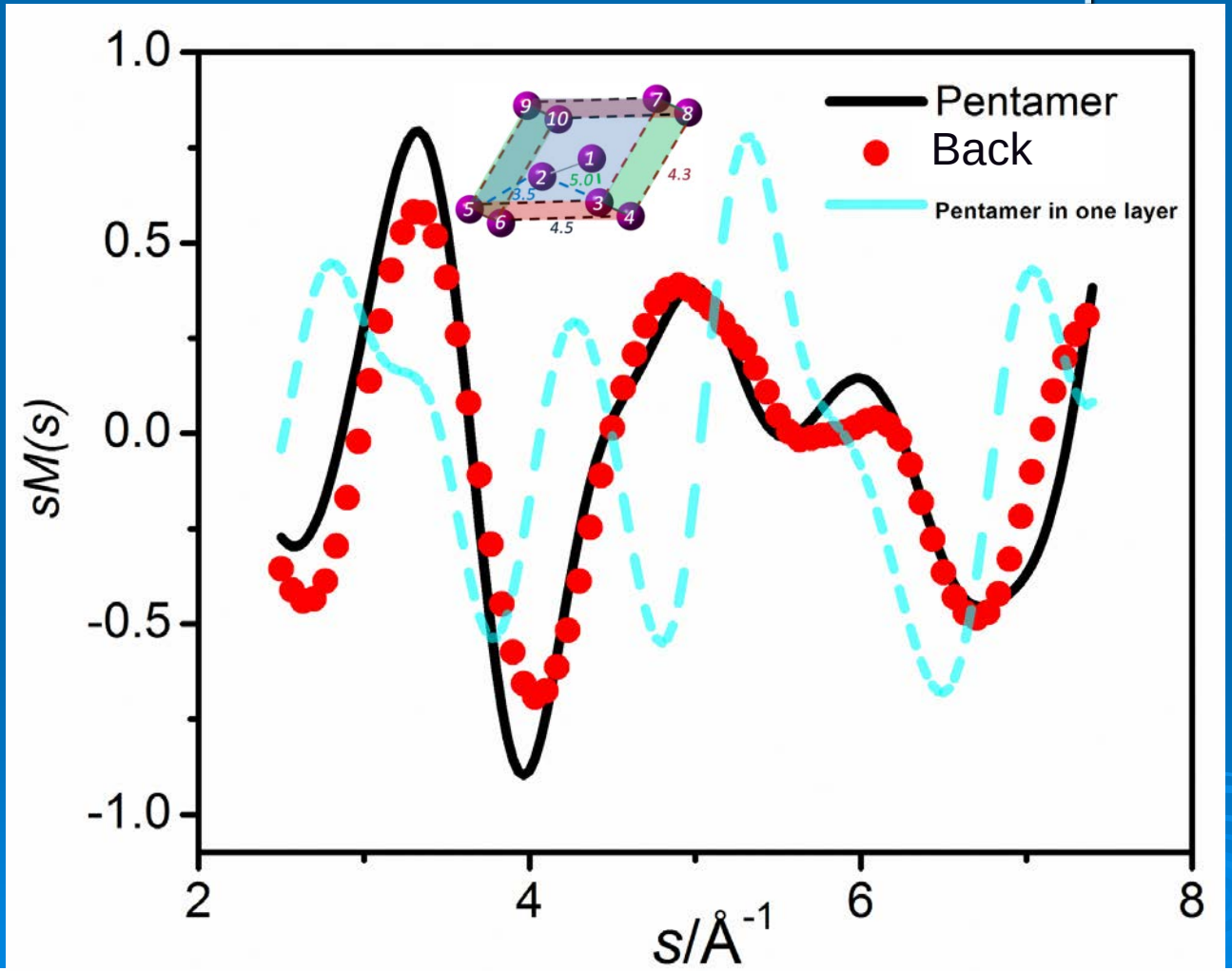


He, Zhang, Lei, and Kong, Angew. Chem. Int. Ed. **56**, 3541 (2017)

Diffraction HALF

Electron diffraction of iodine in droplets



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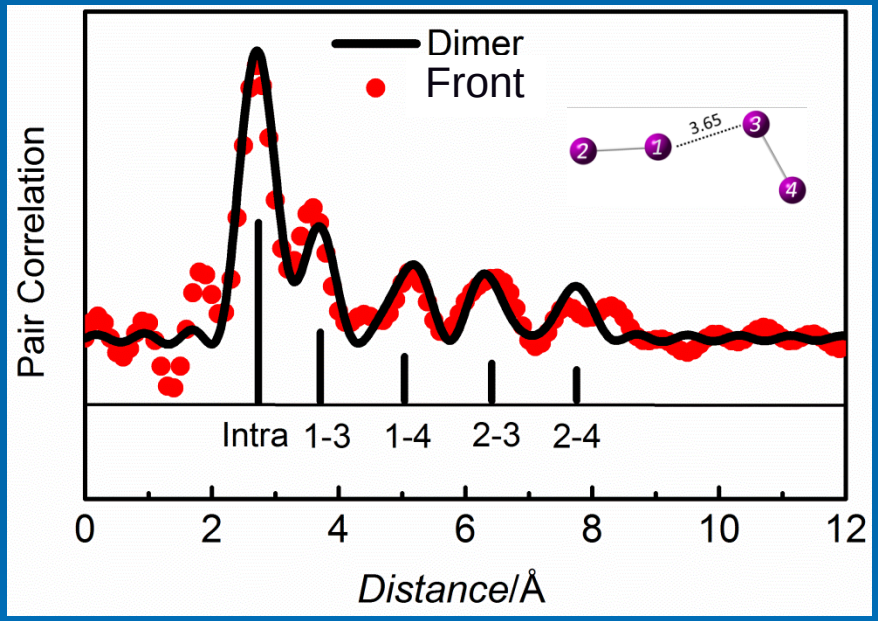
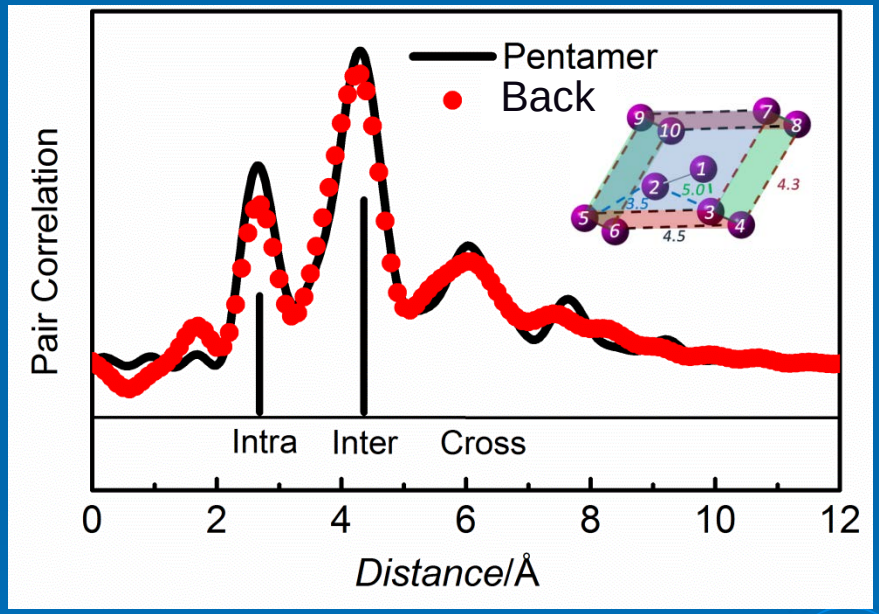
Diffraction Half

Electron diffraction of iodine in droplets

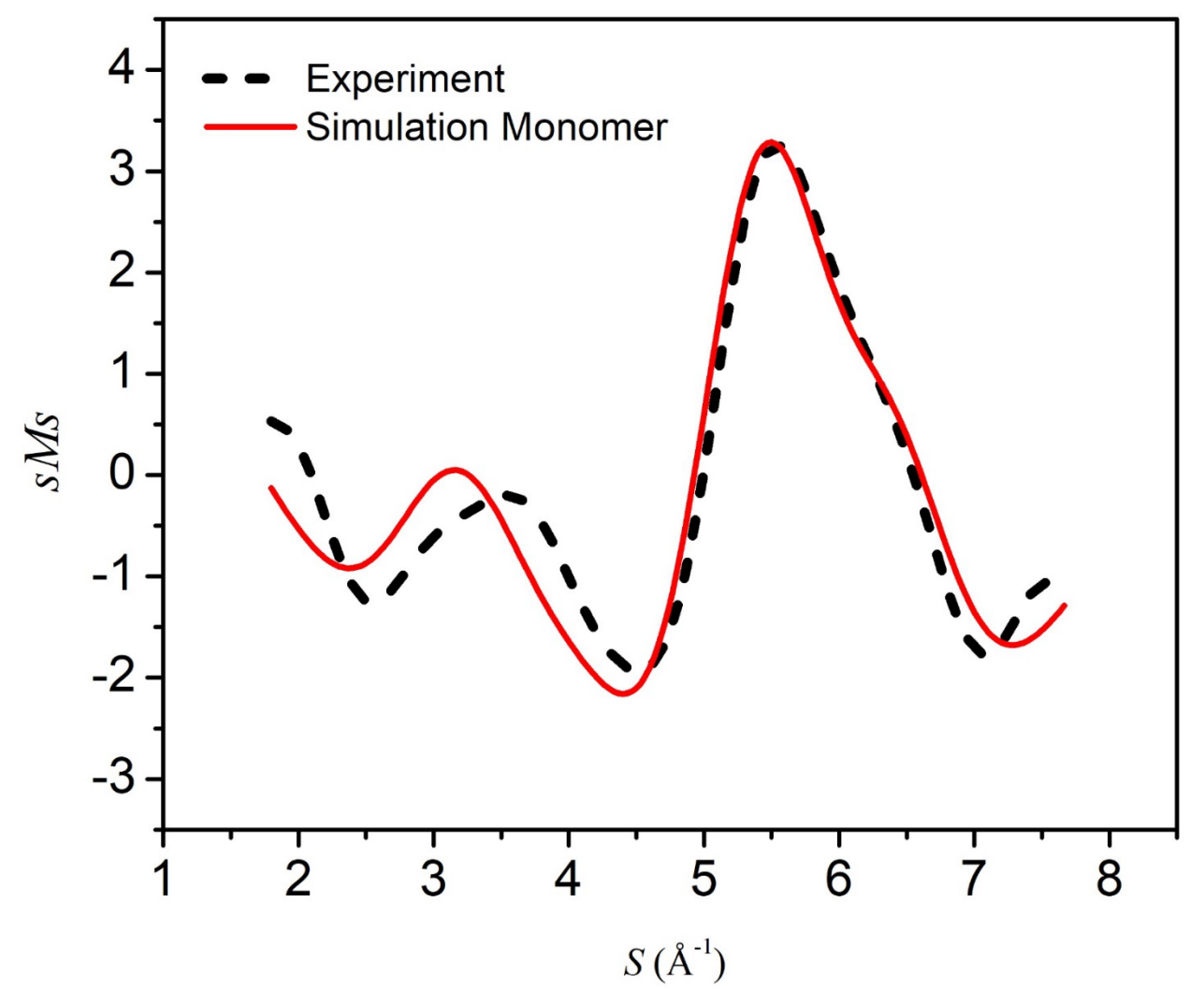




He, Zhang, Lei, and Kong, Angew. Chem. Int. Ed. **56**, 3541 (2017)

Diffraction Half

Electron diffraction of pyrene in droplets



Isomers of pyrene dimer

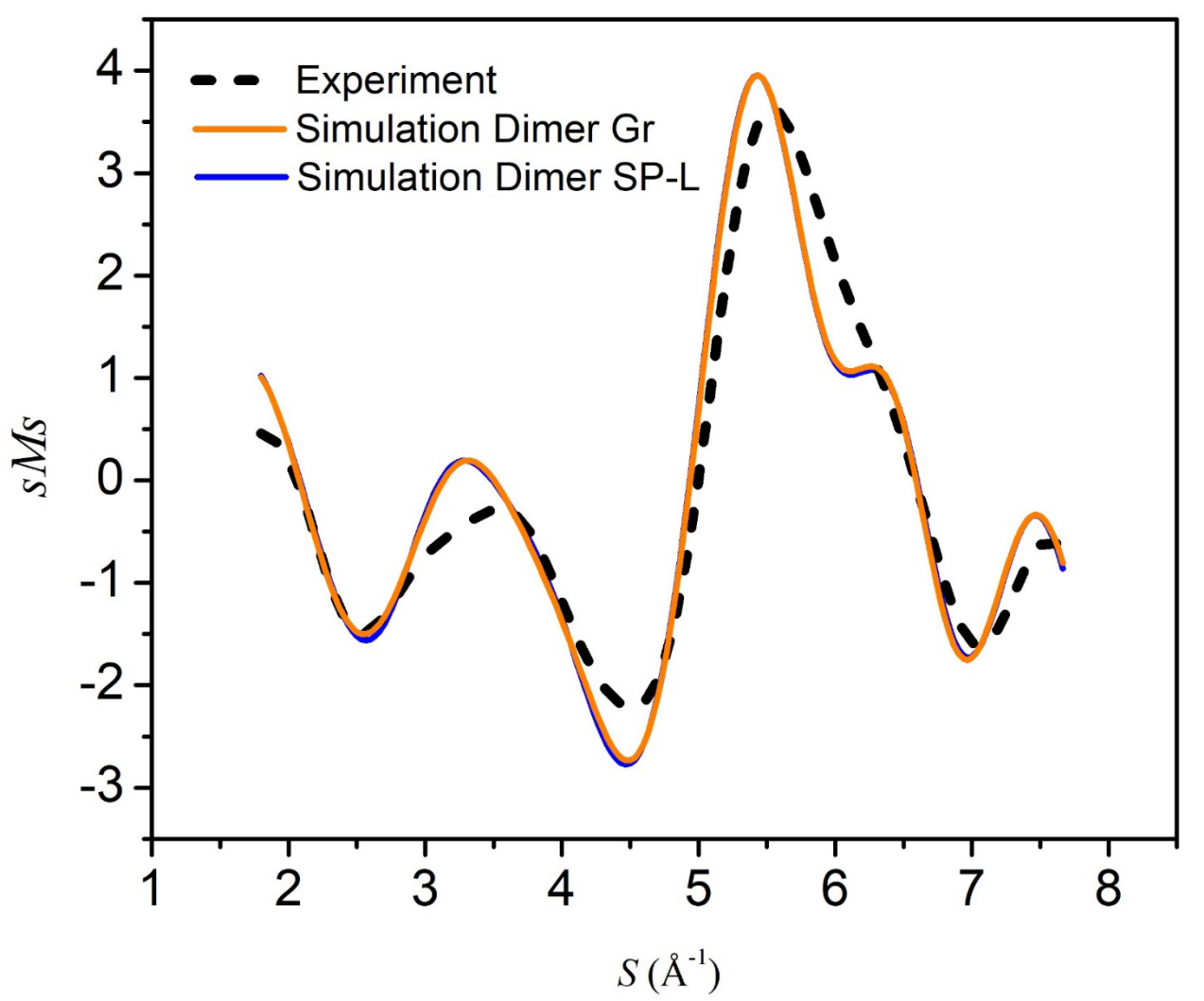
Slipped Parallel (SP-L)

Graphite type (Gr)

Slipped Parallel (SP-S)

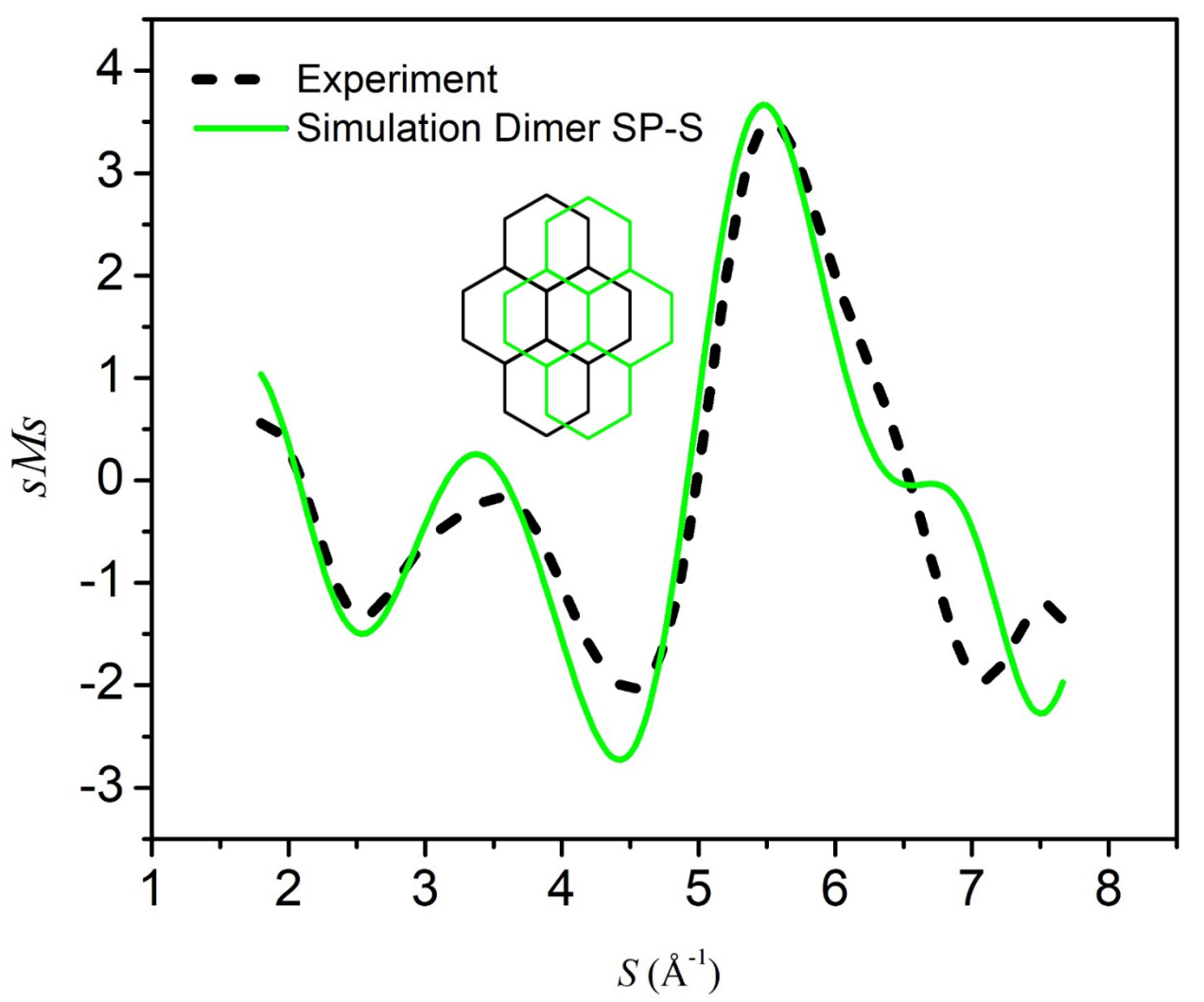
Diffraction Half

Electron diffraction of pyrene in droplets



Diffraction Half

Electron diffraction of pyrene in droplets



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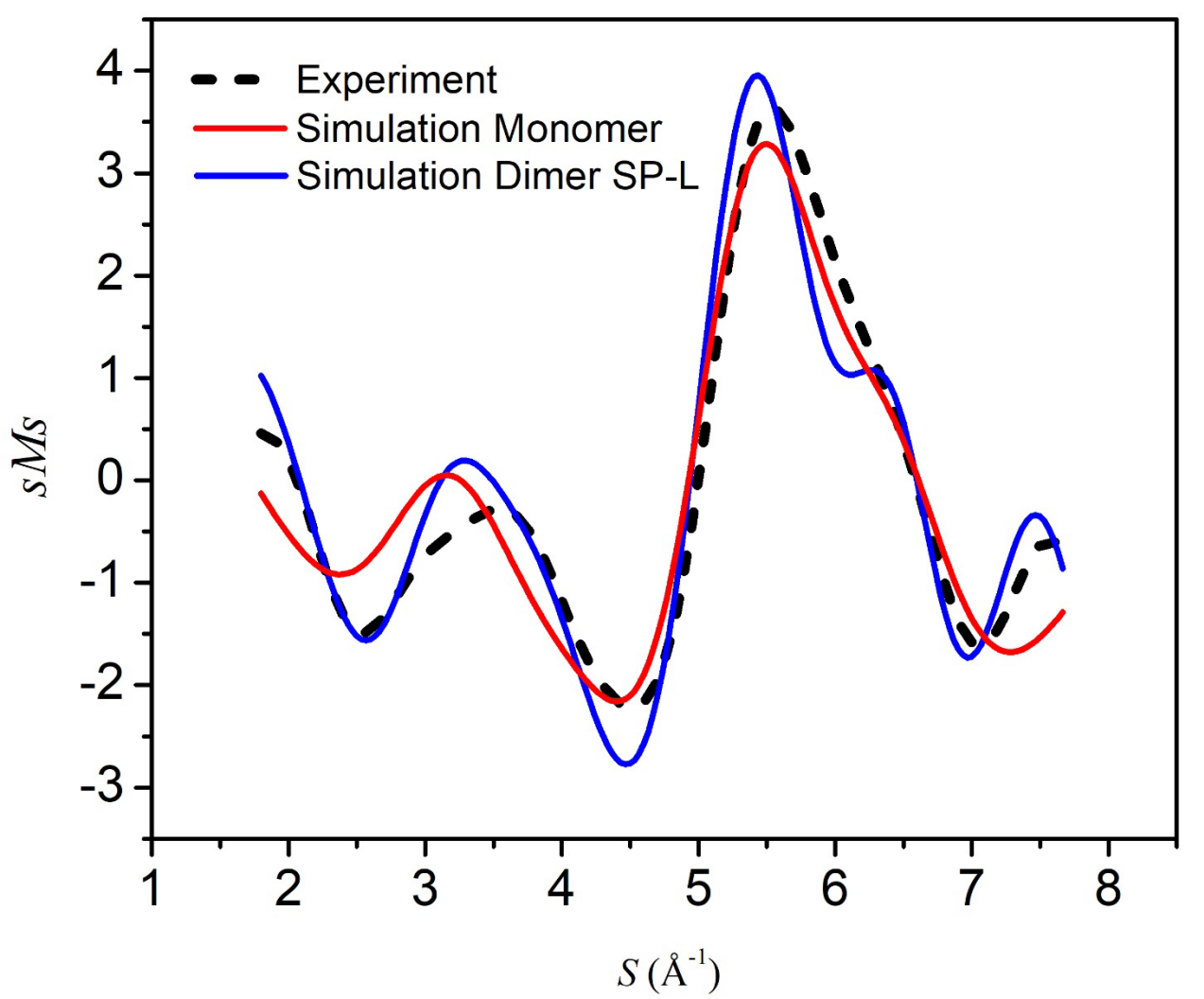
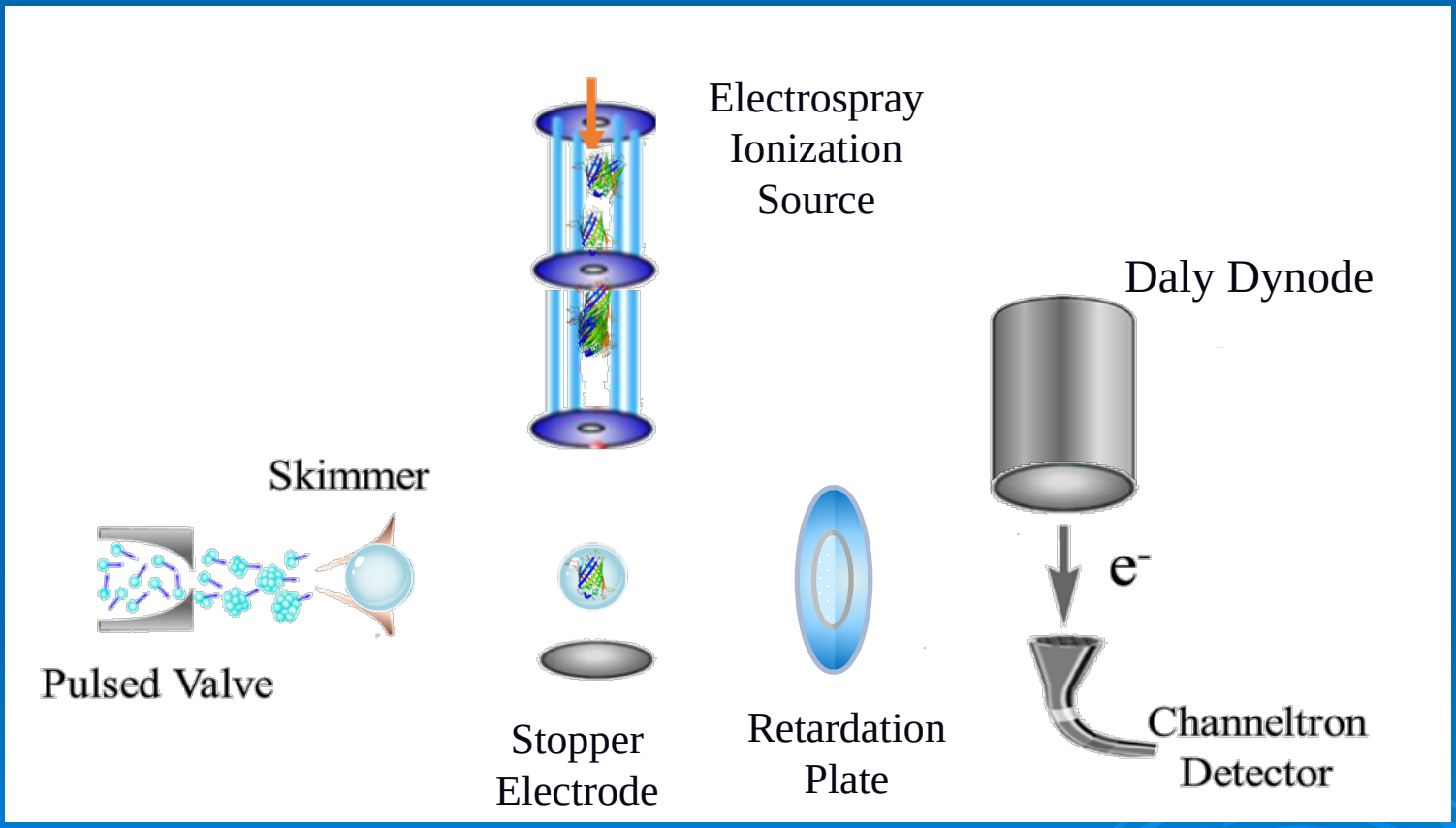


Protein Half: GFP in Droplets



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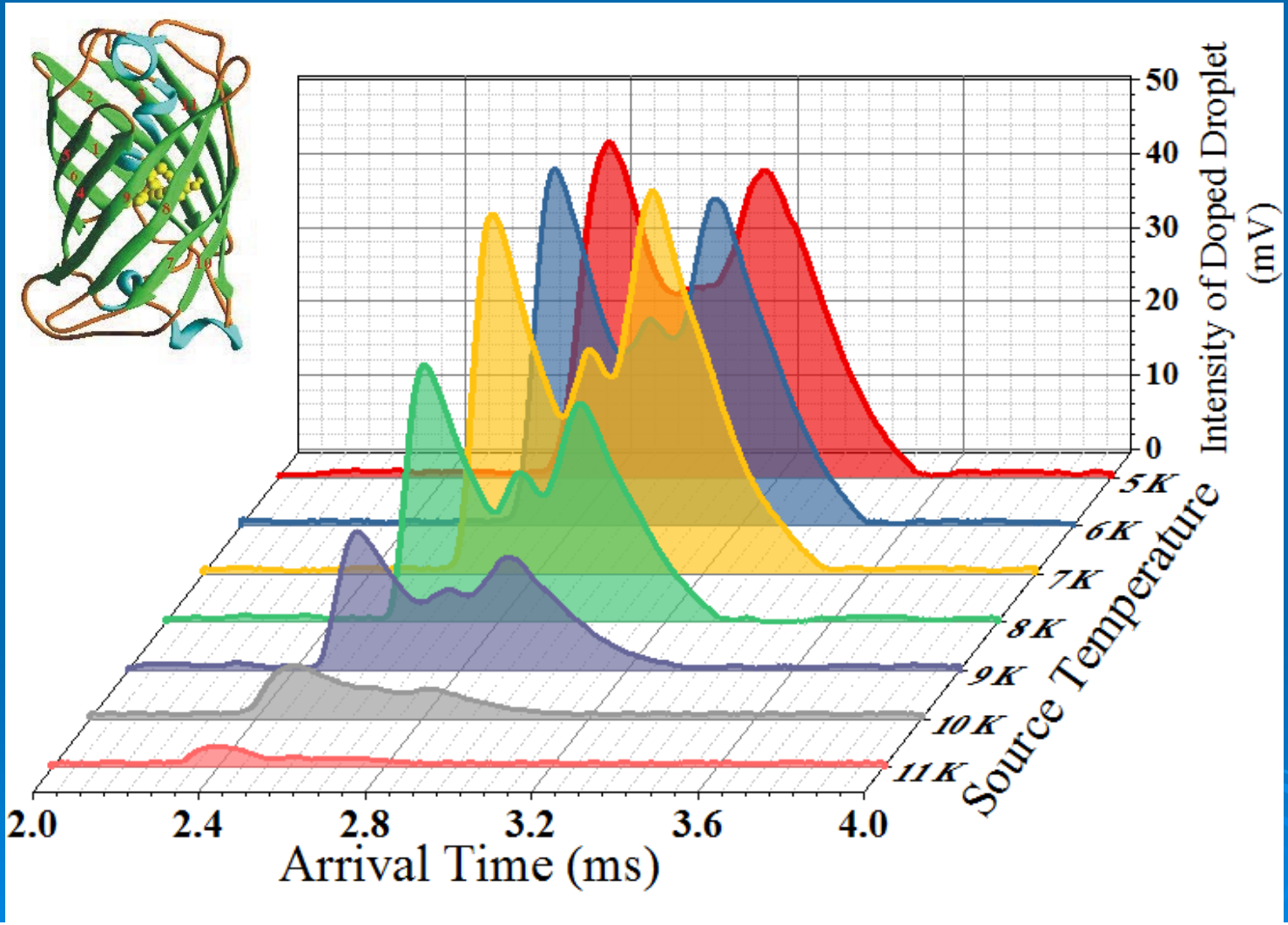
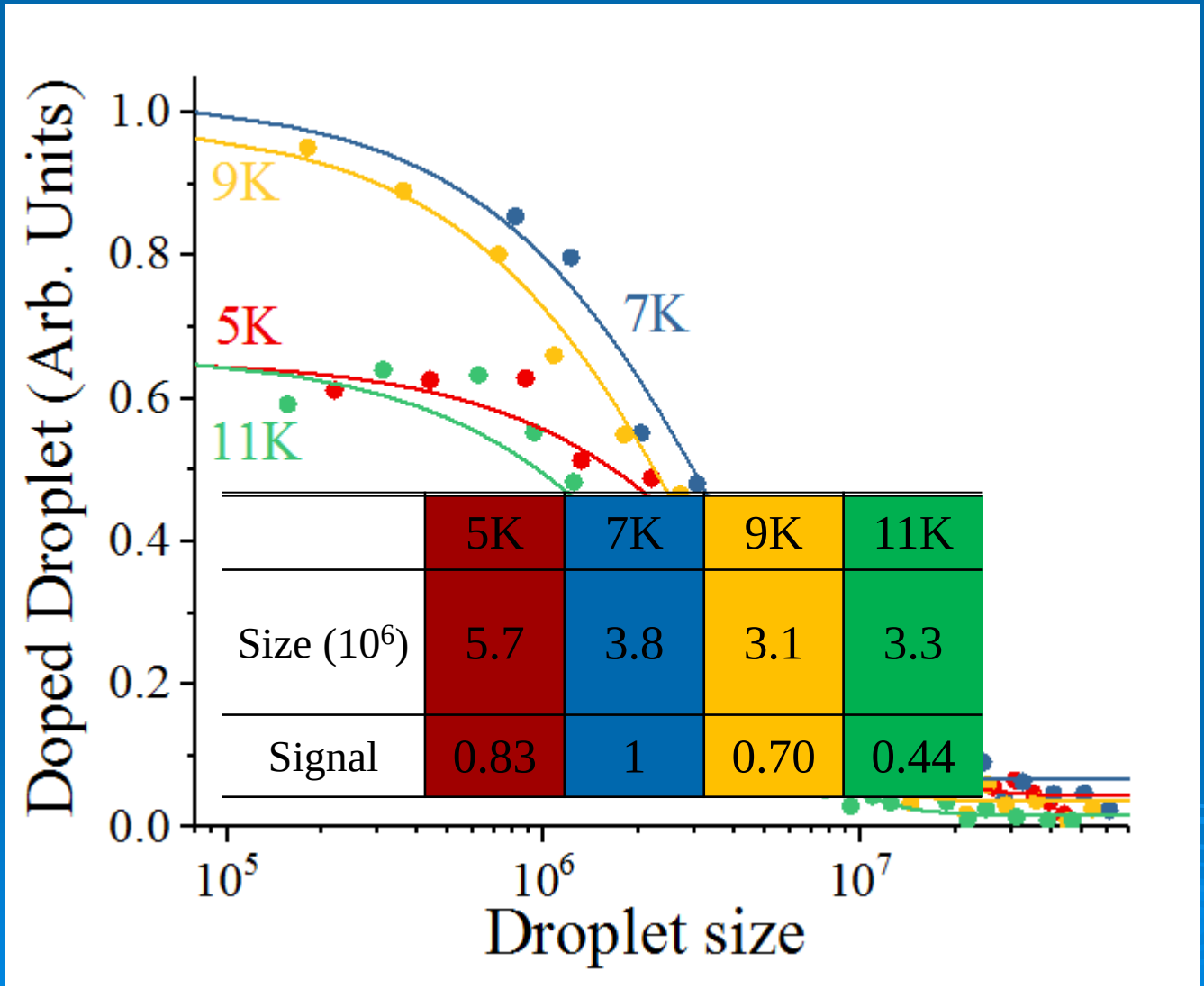


Alghamdi, Zhang, Oswalt, Porter, Mehl, and Kong, J. Phys. Chem. A **121**, 6671 (2017).

Protein Half: GFP in Droplets

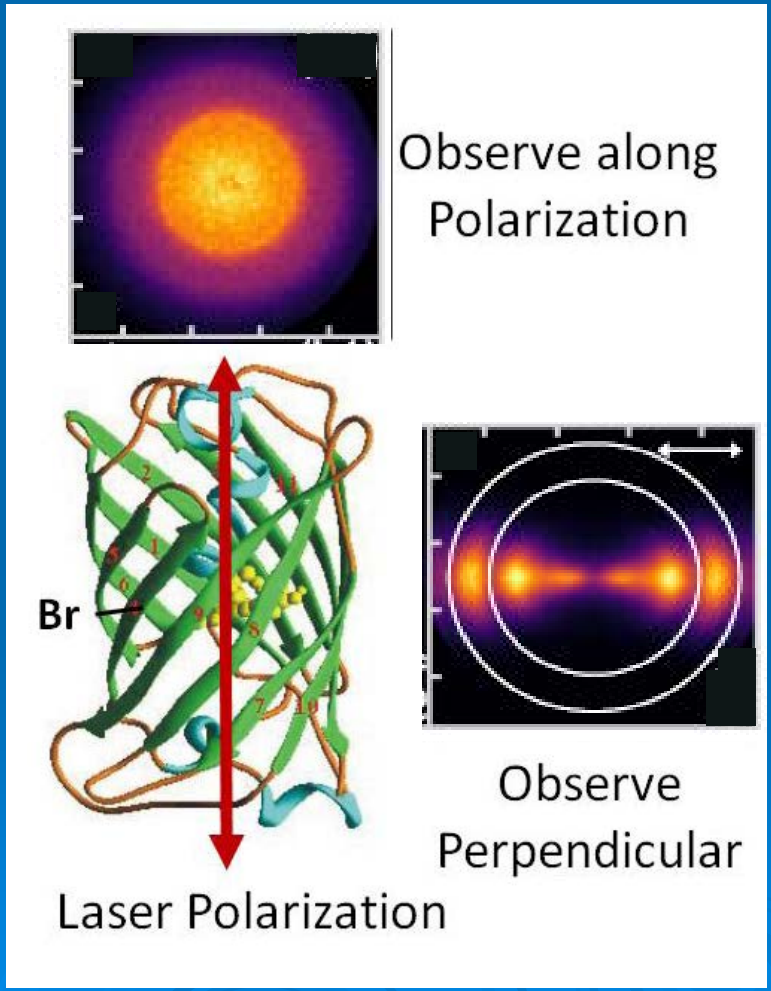


	5K	7K	9K	11K
Size (10^6)	5.7	3.8	3.1	3.3
Signal	0.83	1	0.70	0.44

Alghamdi, Zhang, Oswalt, Porter, Mehl, and Kong, J. Phys. Chem. A **121**, 6671 (2017).

Probing Molecular Alignment

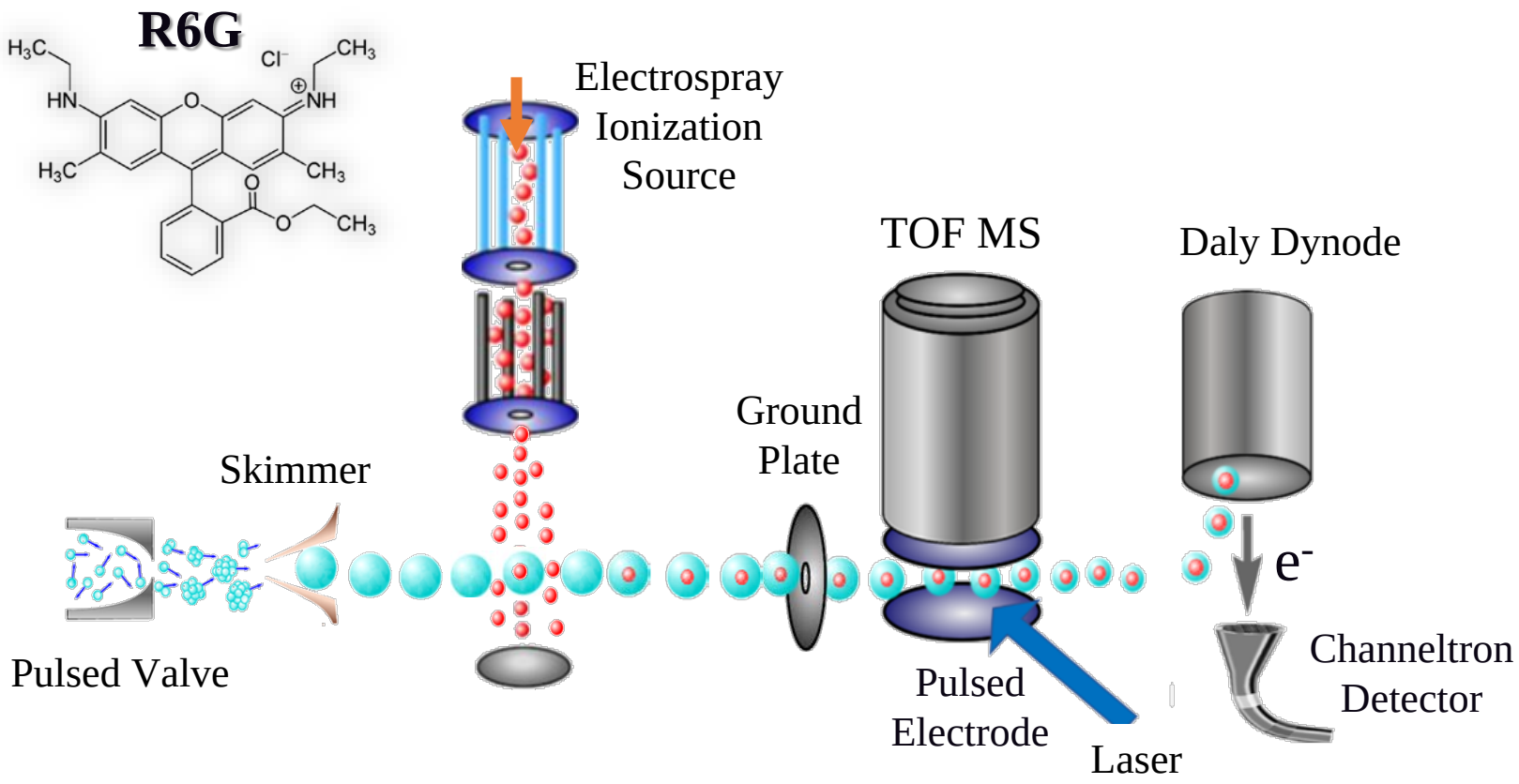
Alignment of doped GFP: Fluorescence and ionization



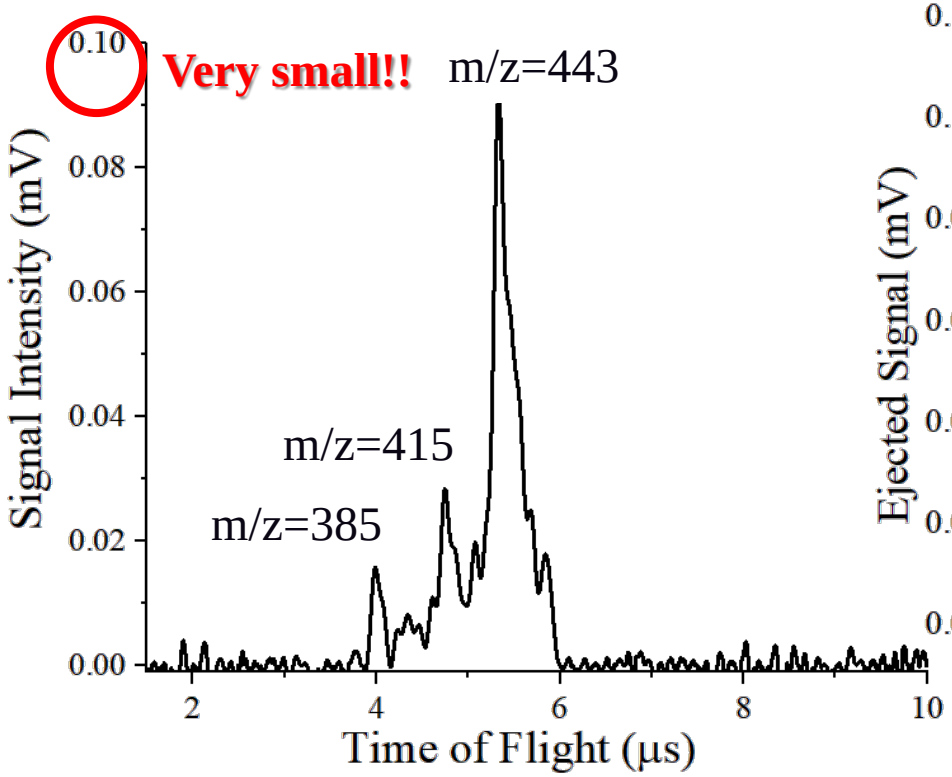
Ryan Mehl
Unnatural Protein Facility

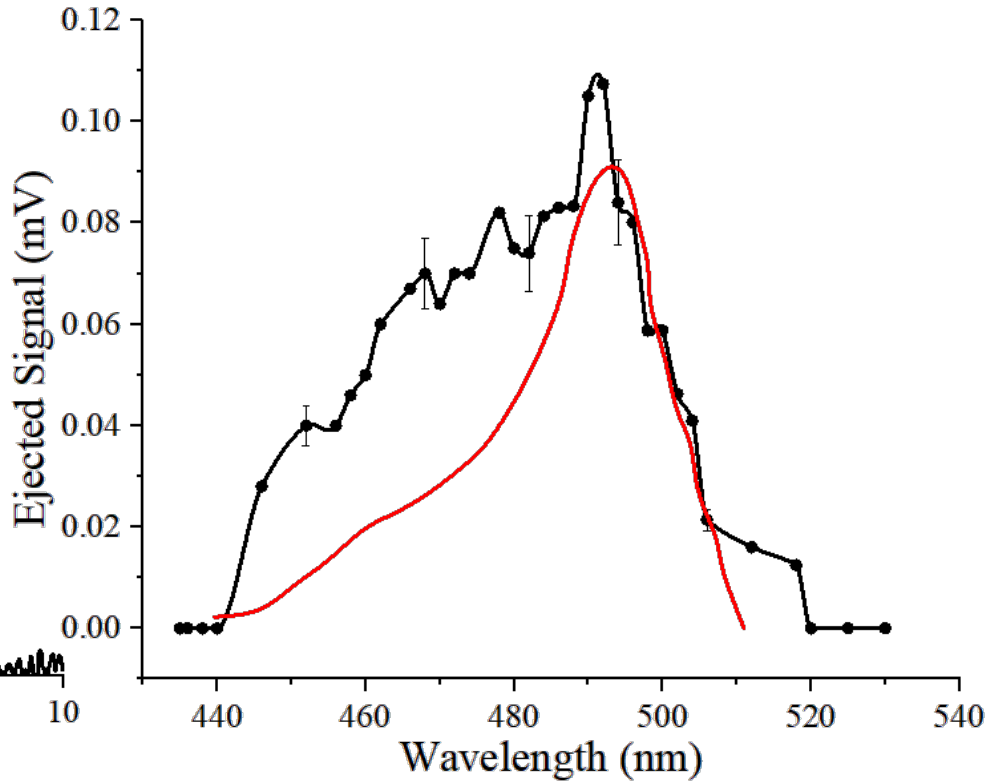
Supplementary funding from NIH: New femtosecond laser for Coulomb Explosion

Nonthermal Ejection



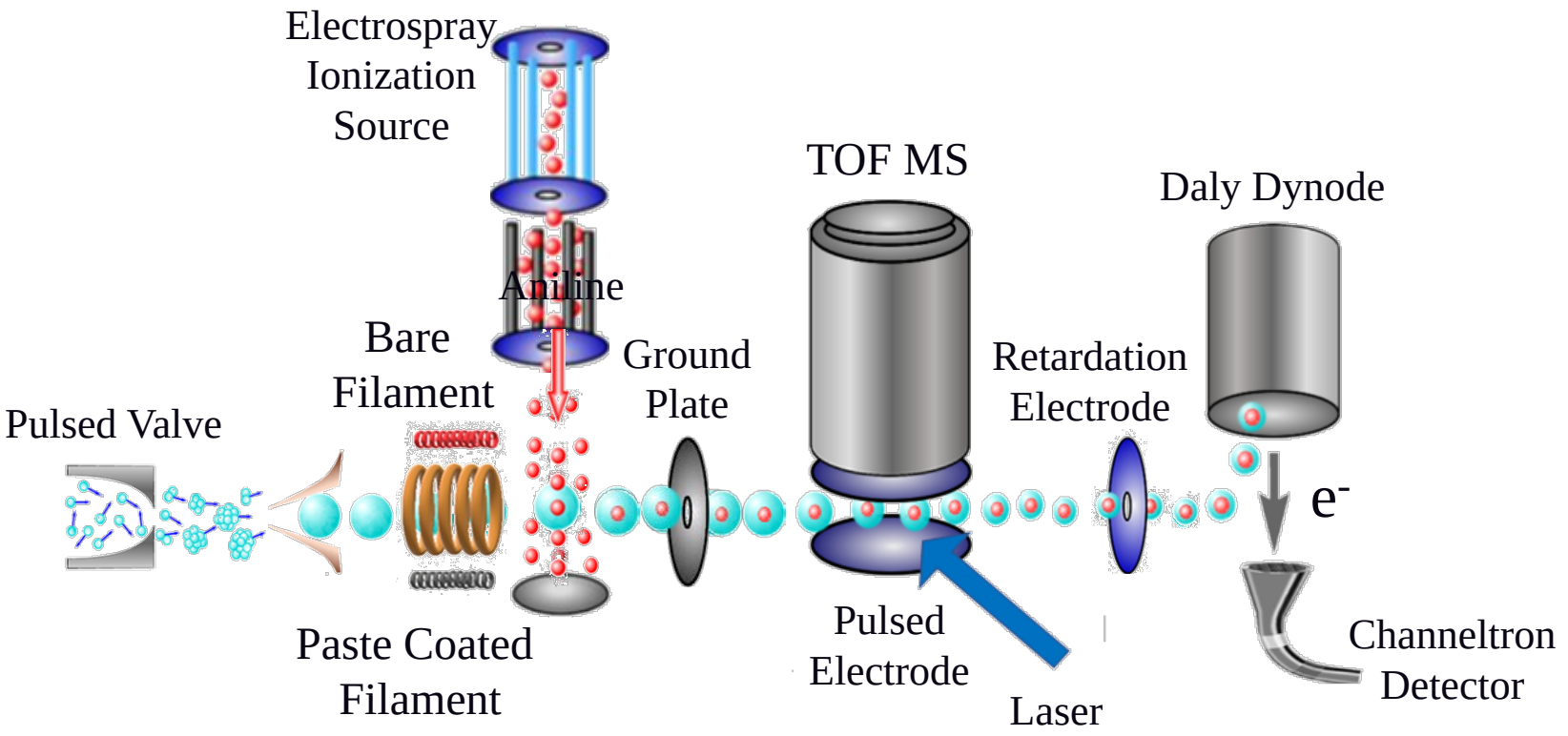
Nonthermal Ejection of R6G





Forbes, M. W., & Jockusch, R. A. (2011)

Nonthermal Ejection of Aniline



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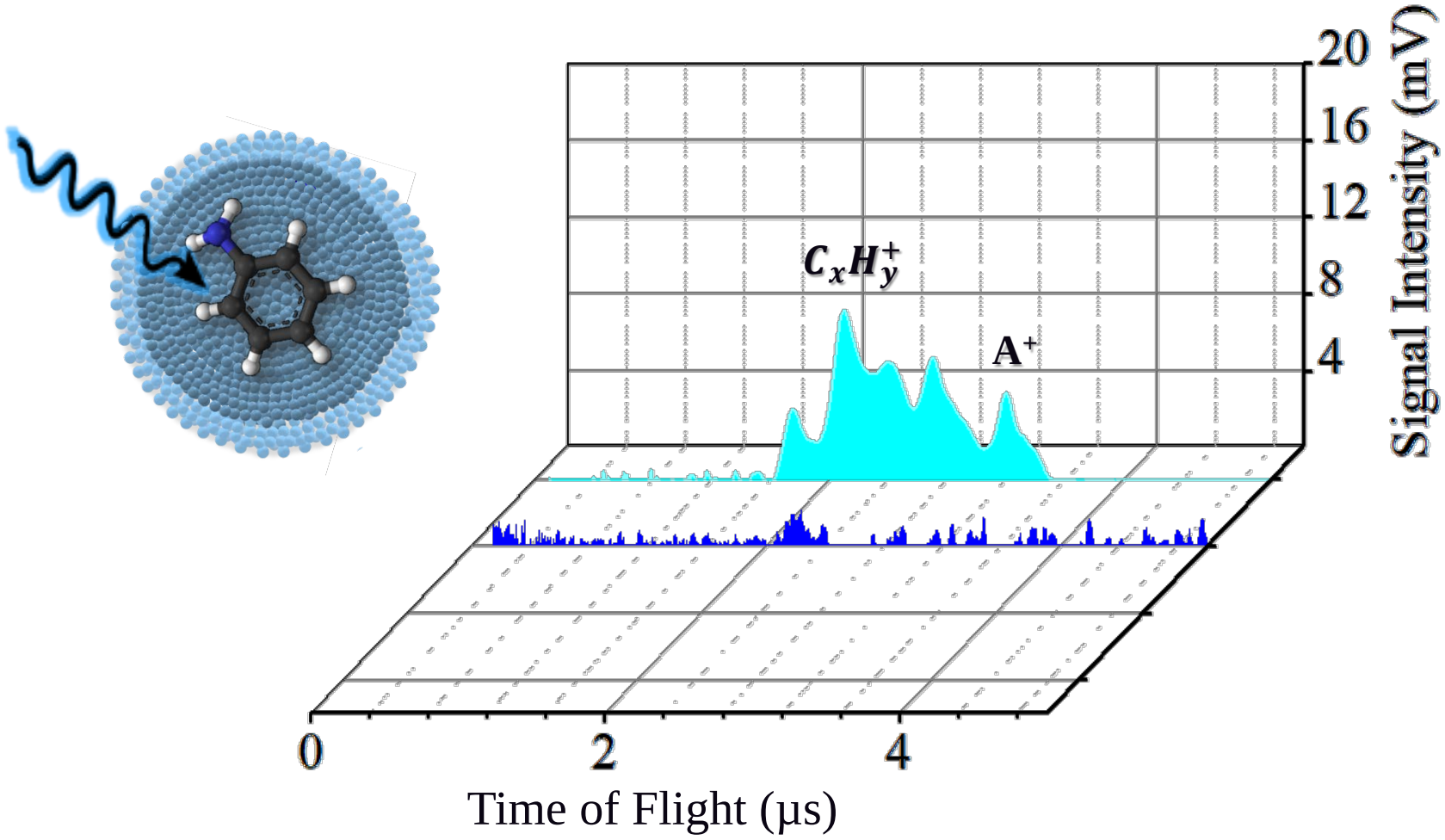

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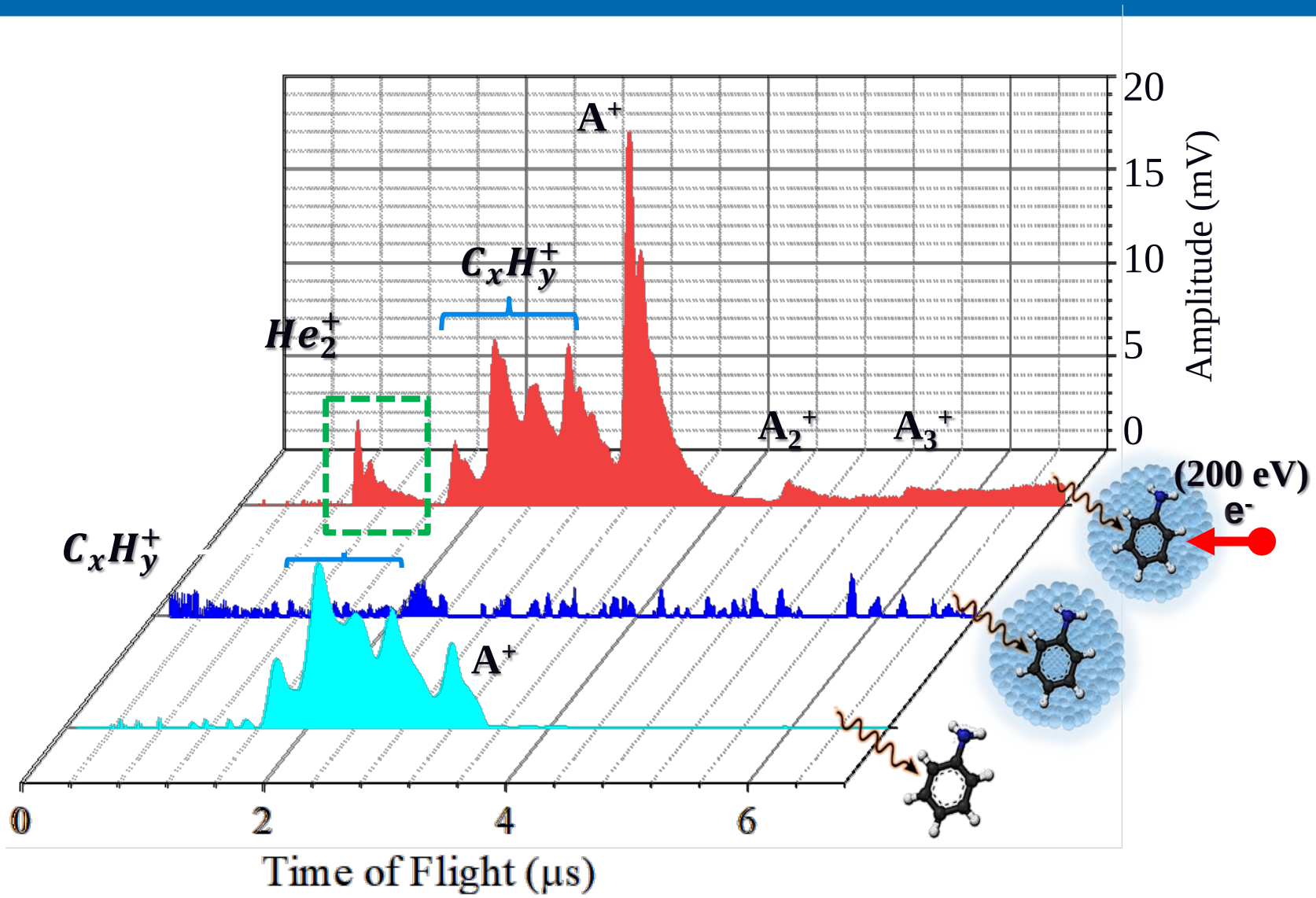

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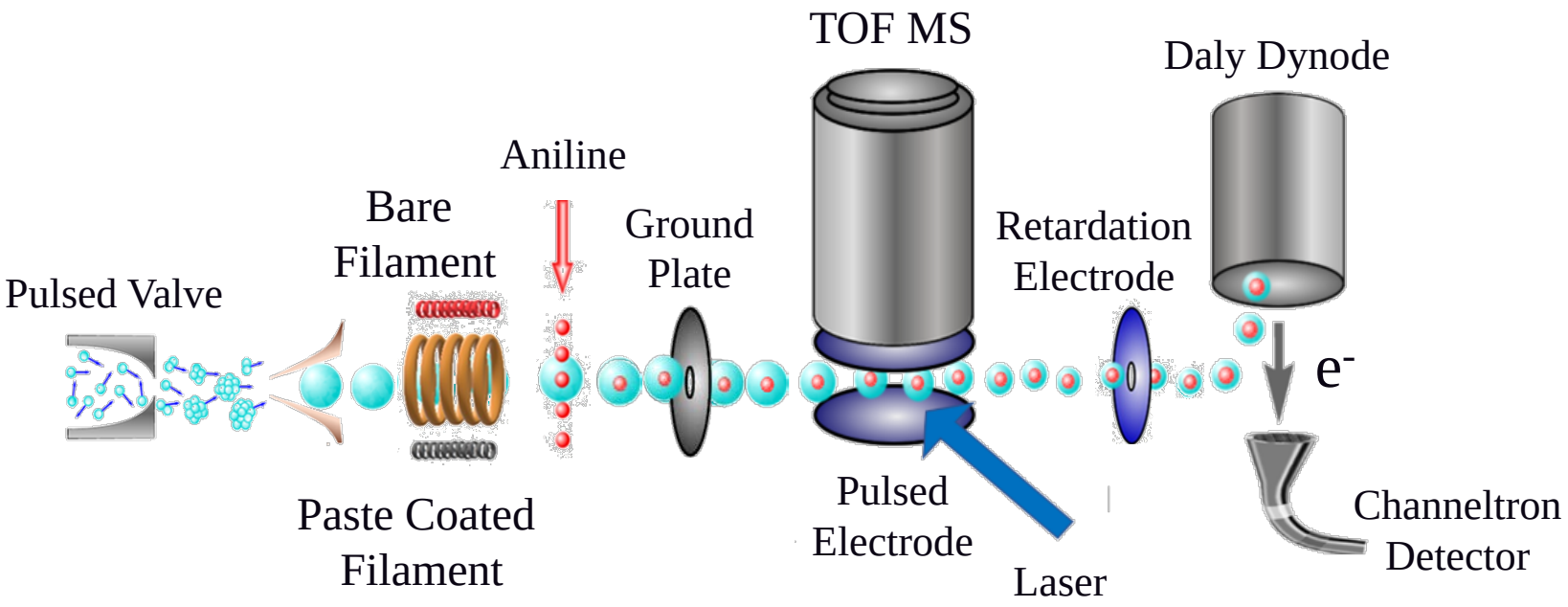

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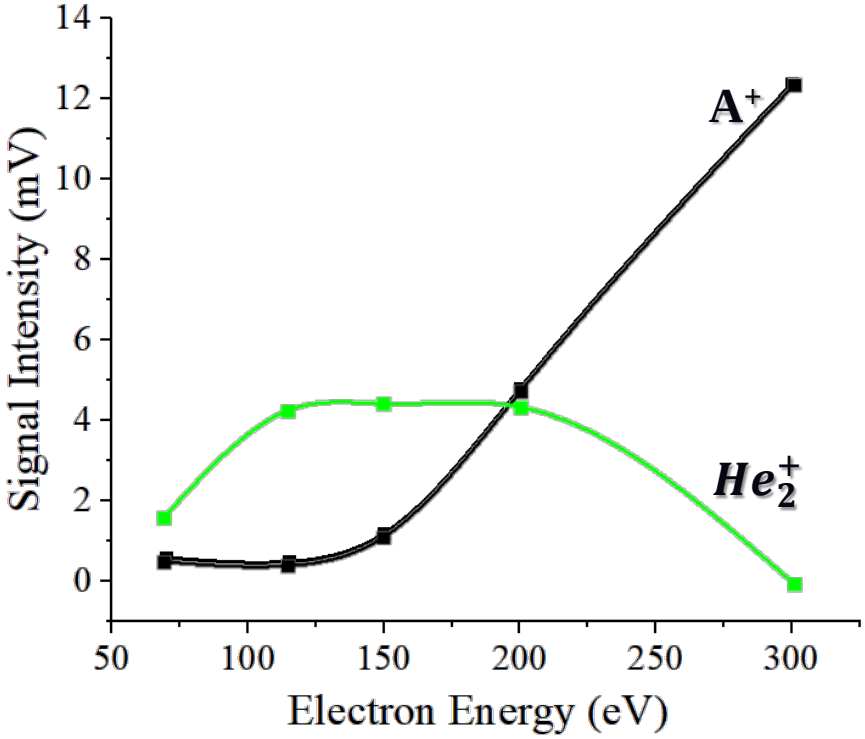

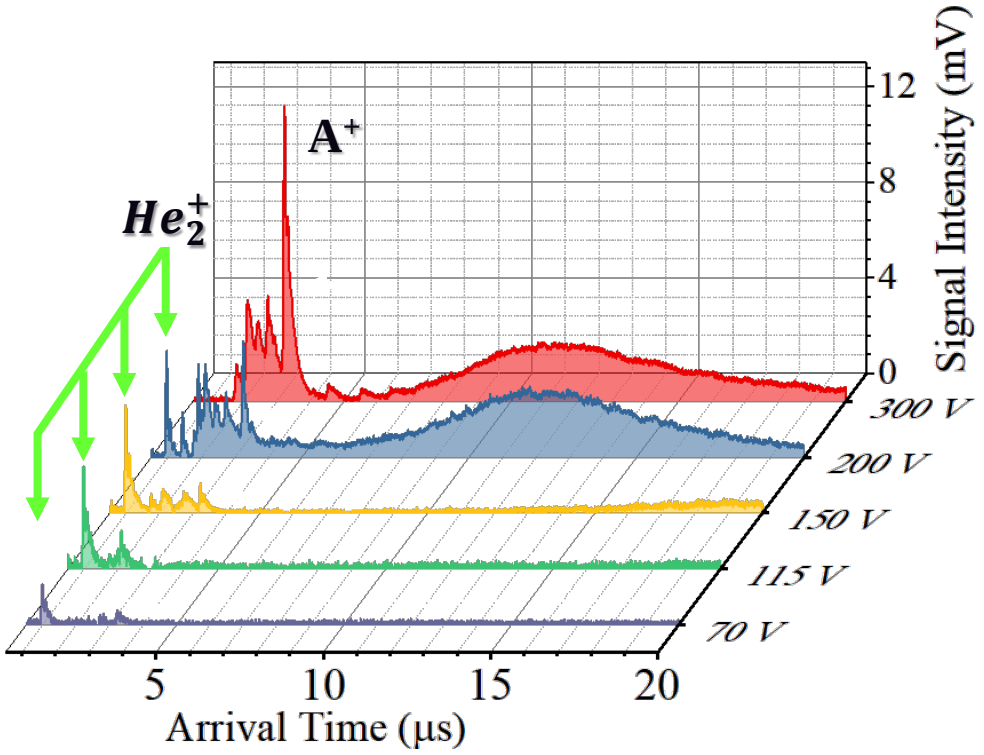

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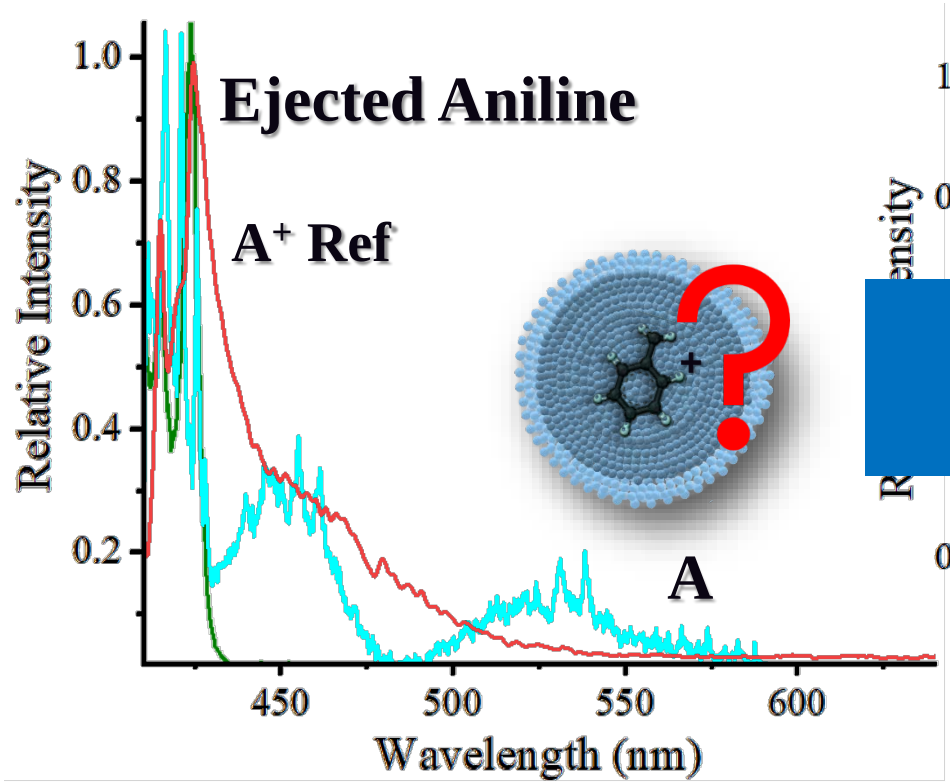
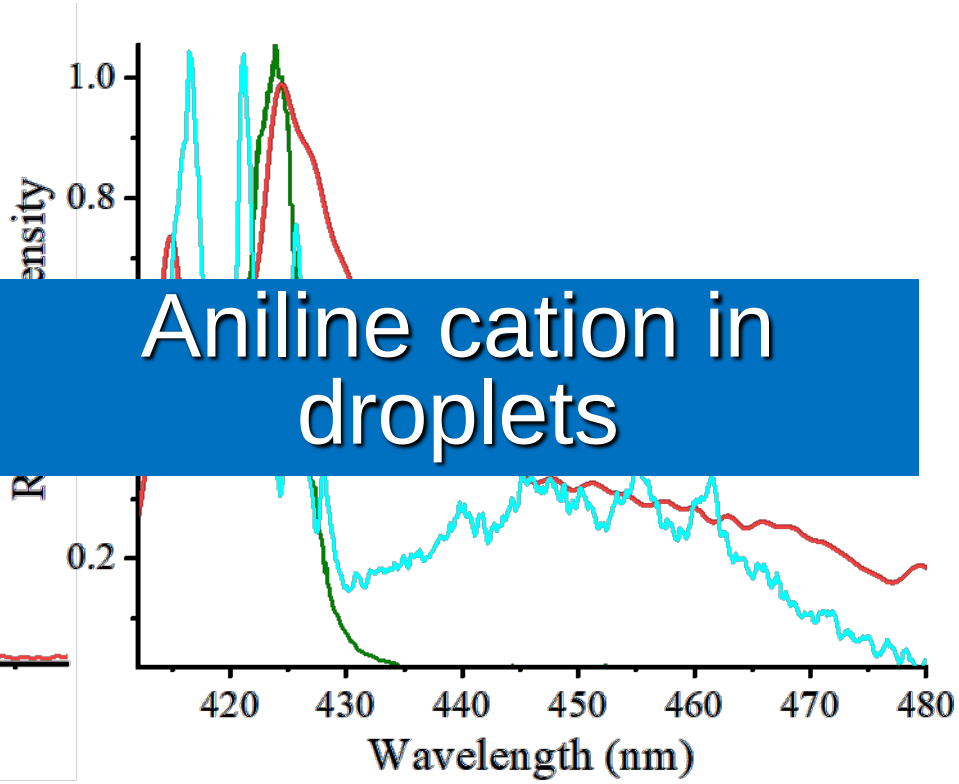


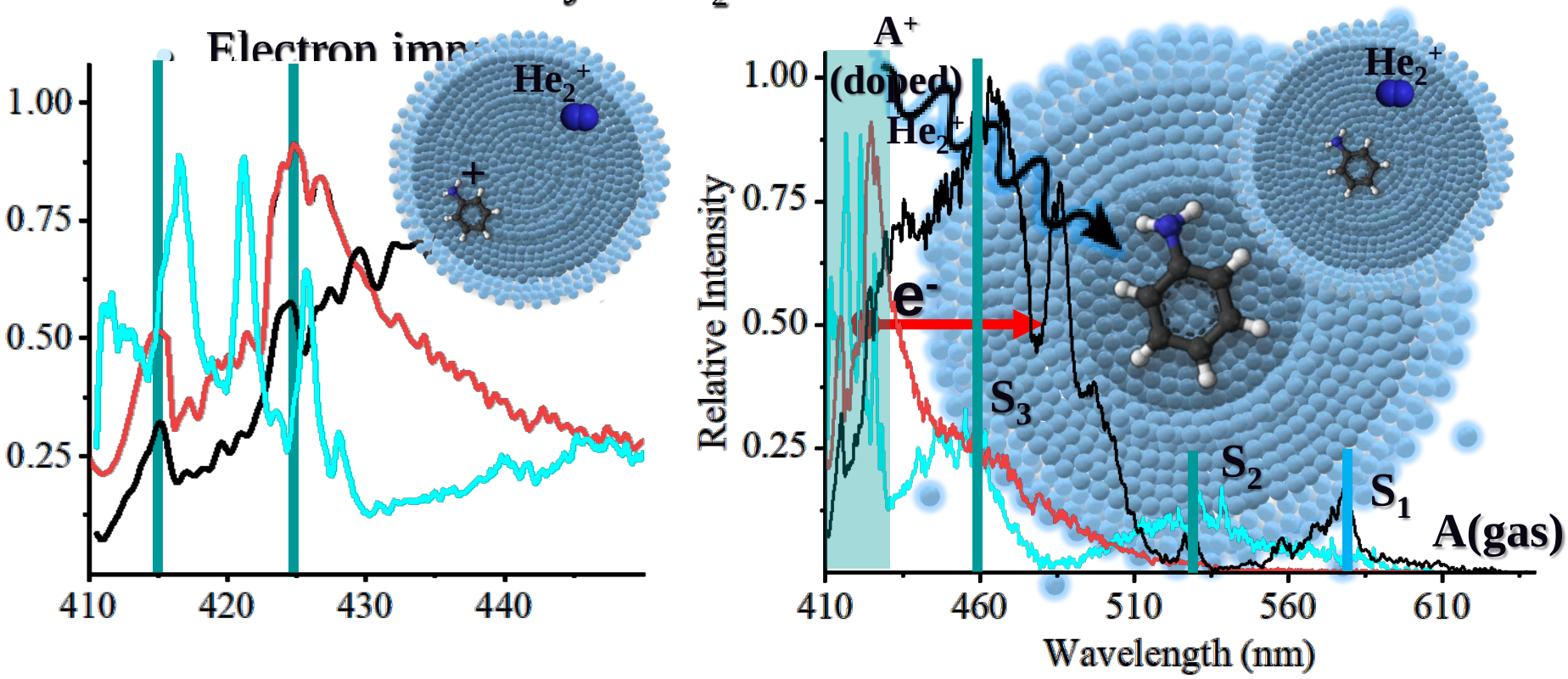


Aniline cation in droplets

Brauer, N. B., Smolarek, S., Zhang, X., Buma, W. J., & Drabbels, M. (2011)

Nonthermal Ejection of Aniline

- Three conditions to eject He_2^+
  - Electron impact



Size matters!

- Small droplets ($<10^5$): gas like
- Large droplets ($>10^6$): bulk like
  - Suppression of MPI
  - Multiple charges in one droplet
  - Suppression of charge transfer

Missions to be accomplished

- Reduce size of droplets and try again!
  - Laser alignment
  - Coulomb explosion
- Electron diffraction from ions (bare & doped)
- Electron diffraction from laser aligned ions doped in droplets

Conclusion

- Electron diffraction of neutral mol in helium droplets
- Doping of proteins into droplets
- Size matters
- The journey continues …

The Fearless Crew

Postdoc

Fan Zhang

Robert Kykyneshi

Engineer

Yongsheng Liu

Ph. D

Colin Harthcock (2015)

Lei Chen (2016)

Yunteng He (2017)

Collaborators at OSU: **Ryan Mehl (Unnatural Protein Facility)**
Lan Xue (Statistics)

Special thanks

Professor D. R. Herschbach
Professor J. P. Toennies
The droplet community

Oregon State University

Funding


ONAMI
OREGON NANOSCIENCE AND
ICROTECHNOLOGIES INSTITUTE
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NSF
rdock
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