

Using machine learning to understand time-resolved x-ray absorption spectra.

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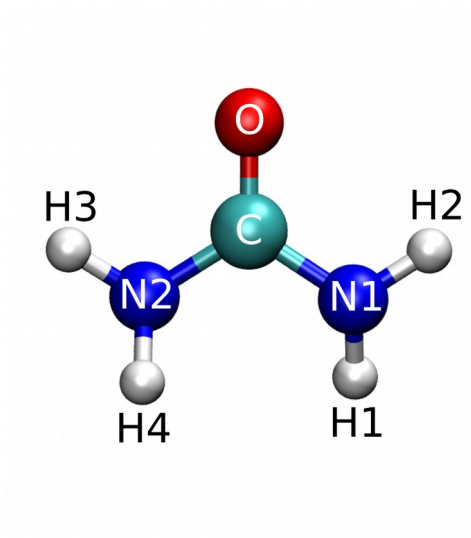
CFEL-DESY Theory Division

and

Universität Hamburg

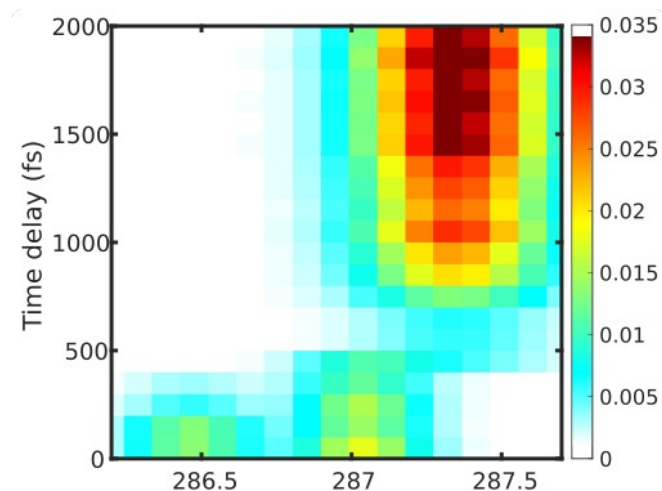
Round Table on AI @DESY, 03.12.2021

Difficulty in interpreting spectra

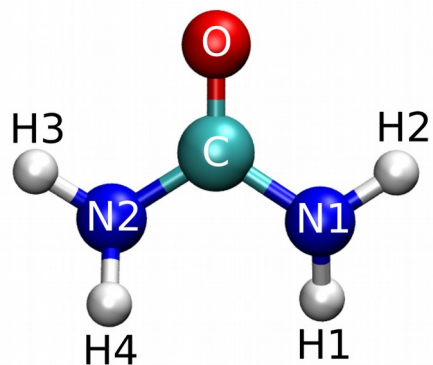


System:
ionized urea

C peak:
Experiment

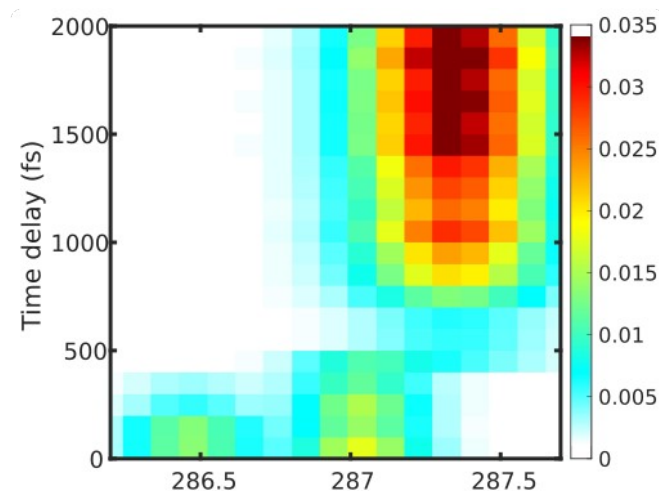


Difficulty in interpreting spectra

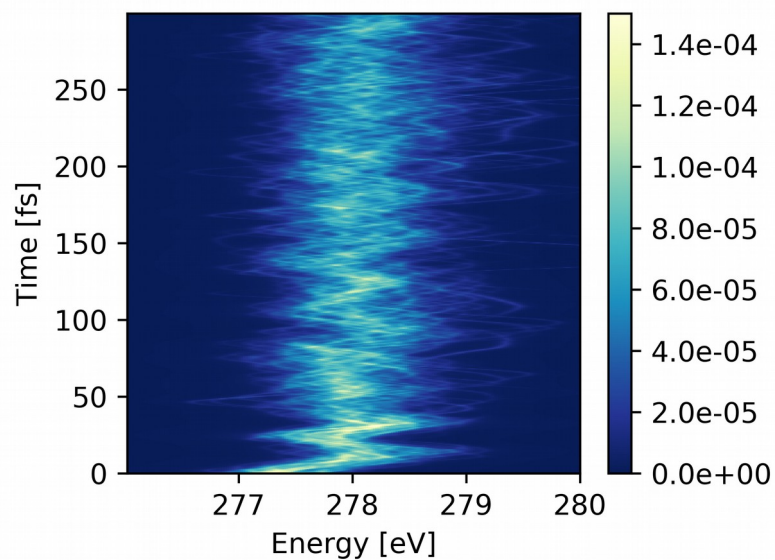


**System:
ionized urea**

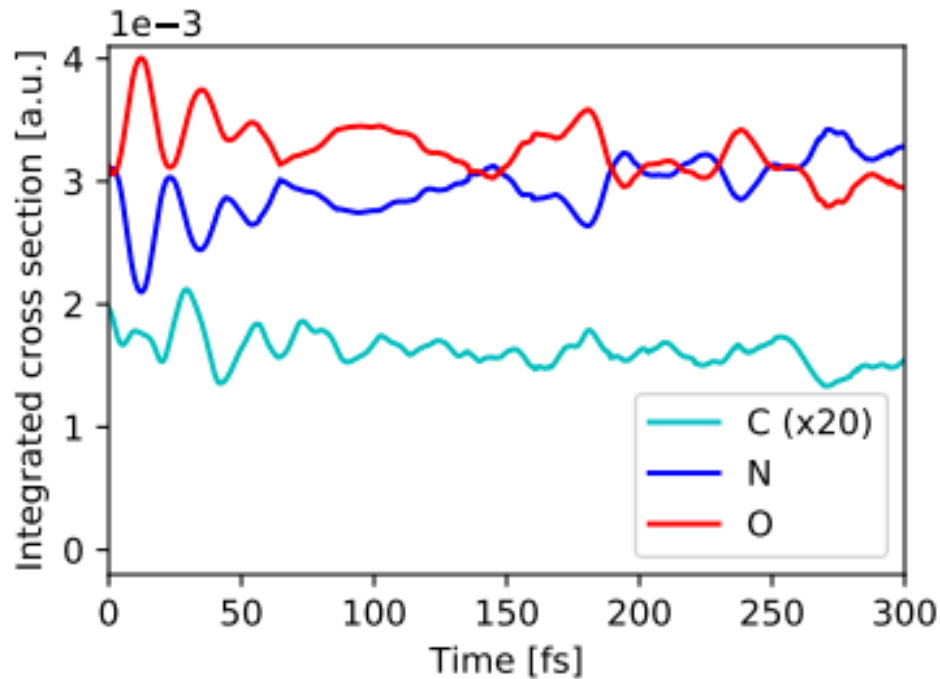
**C peak:
Experiment**



**C peak:
Theory**



Not possible to interpret oscillations



HOMO ionization shows oscillations

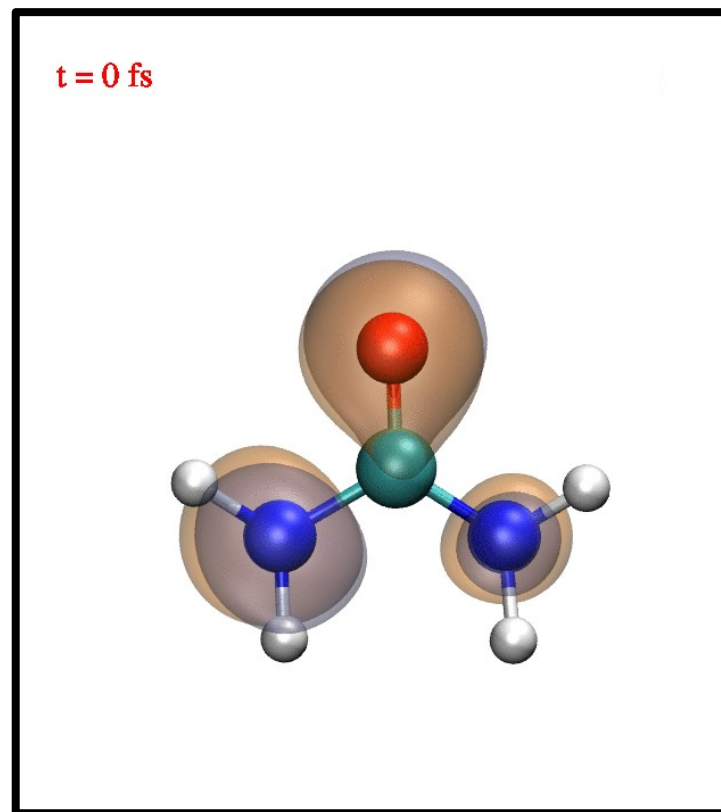
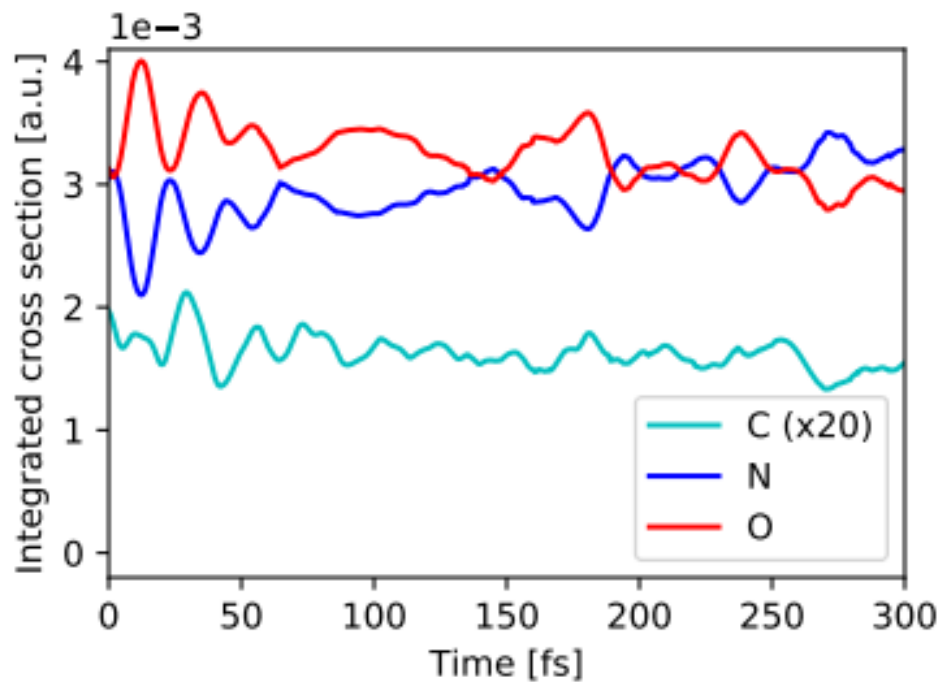
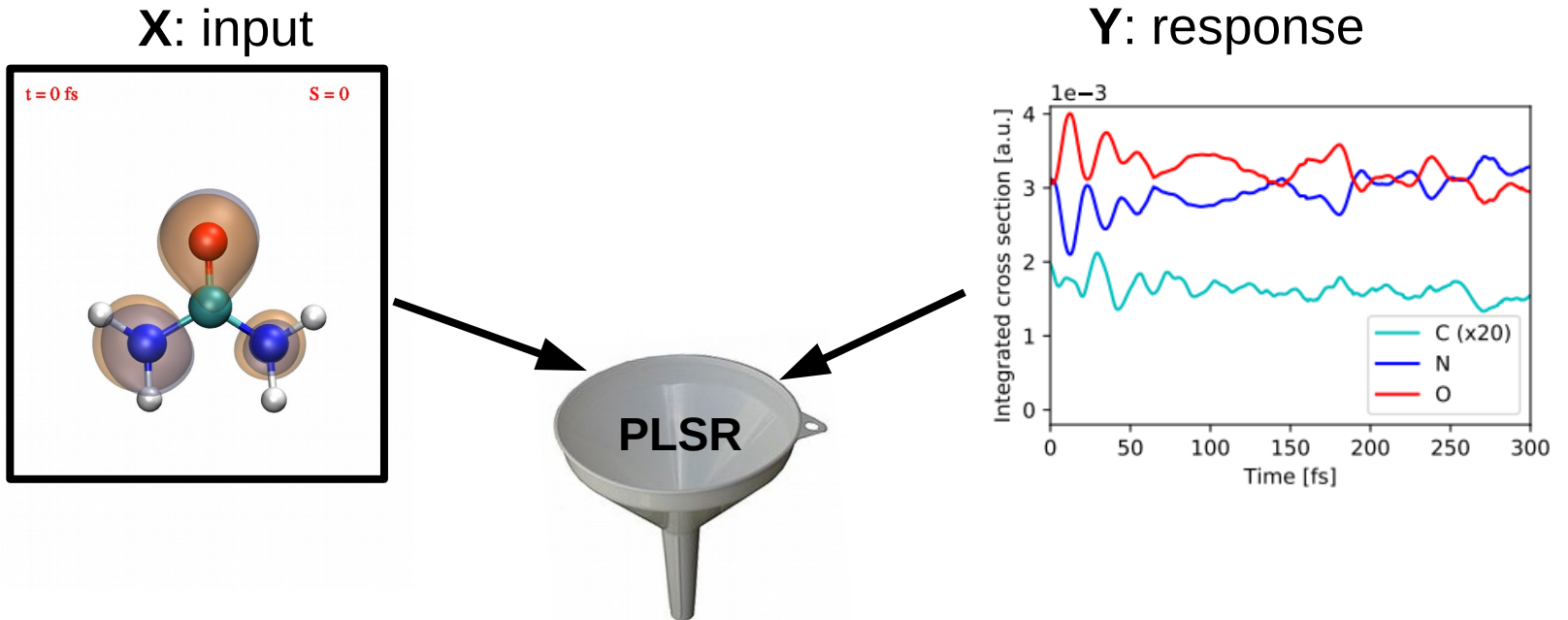


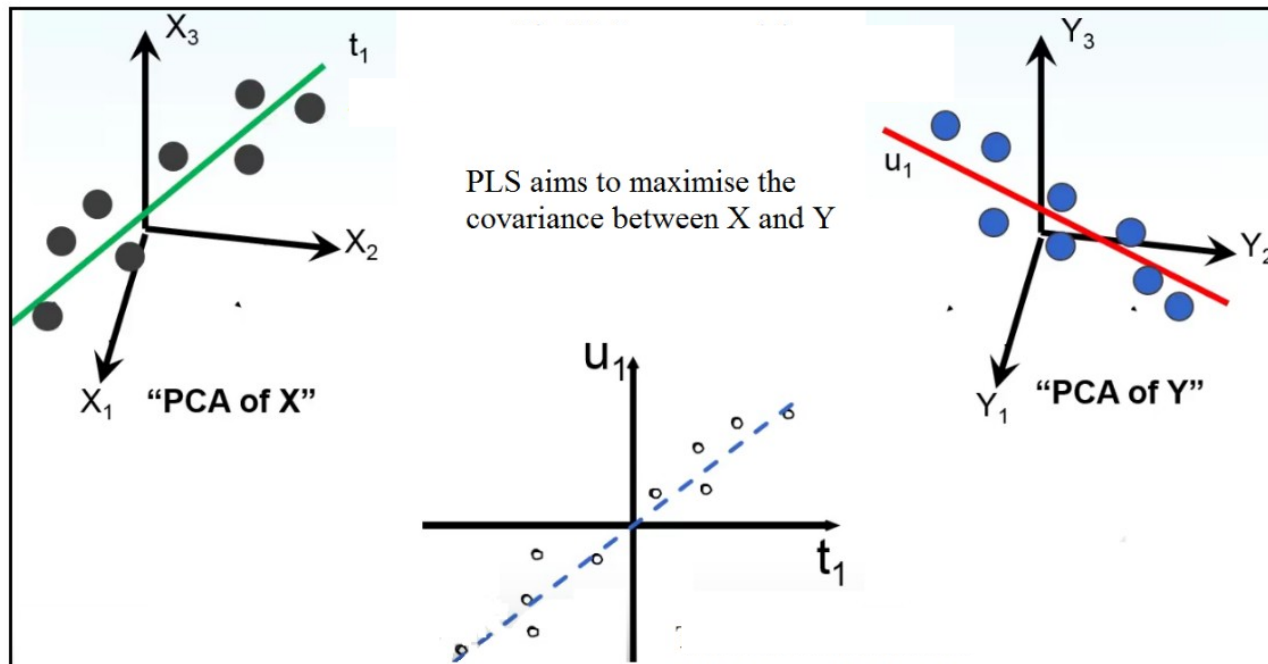
FIG: Dynamics with electron hole density.

Dimensionality reduction using partial least squares regression (PLSR)



Partial least squares regression (PLSR)

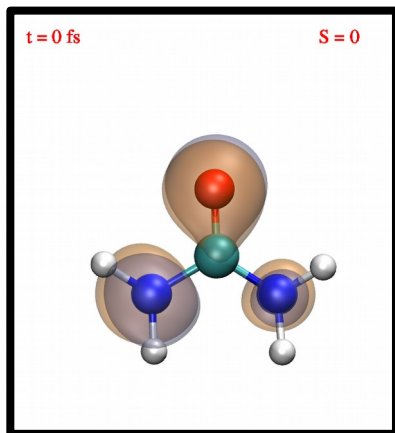
- Dimensionality reduction
- Similar to principle component analysis (PCA)
- But for input (X) and response (Y)



Source: IEEE Sensors Journal, 2018, 18, 6715-6726

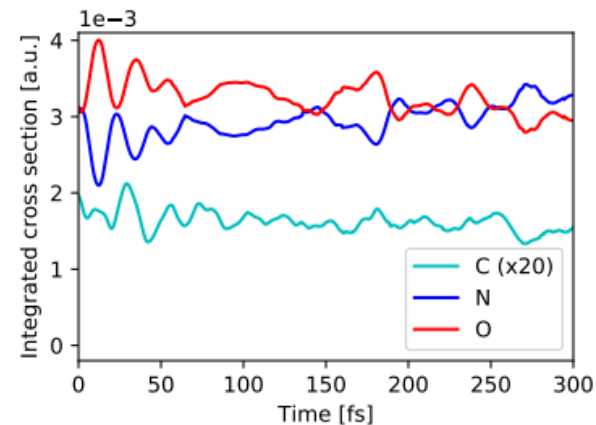
Dimensionality reduction using partial least squares regression (PLSR)

X: input

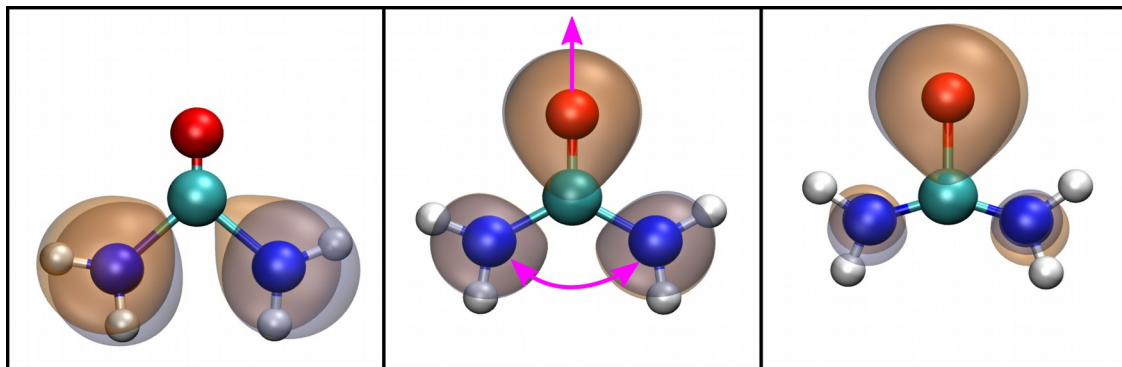


PLSR

Y: response

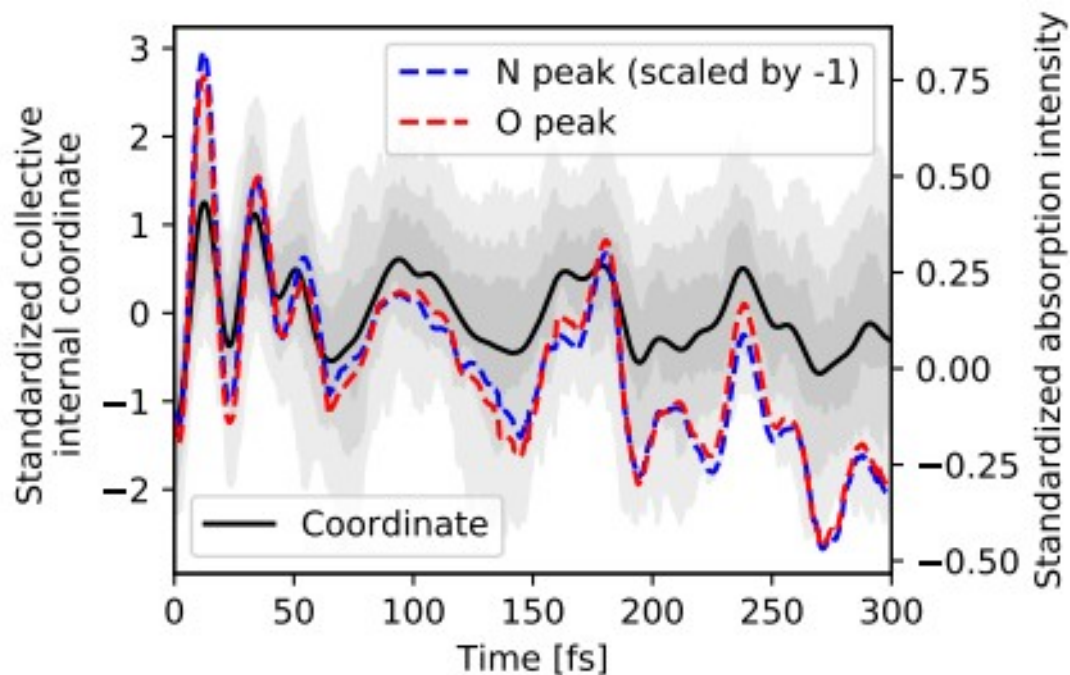
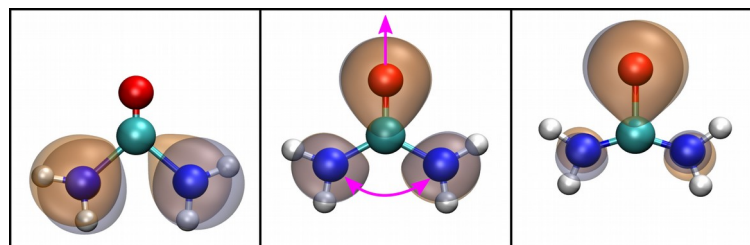


N and O peaks:
 $R^2 = 77\%$



Verifying collective coordinate

N and O peaks: $R^2 = 77\%$



Conclusion

- PLSR reveals collective coordinates for intensity oscillations.

Reference

- Shakya et al., Struct. Dyn. **8**, 034102 (2021)

Conclusion

- PLSR reveals collective coordinates for intensity oscillations.

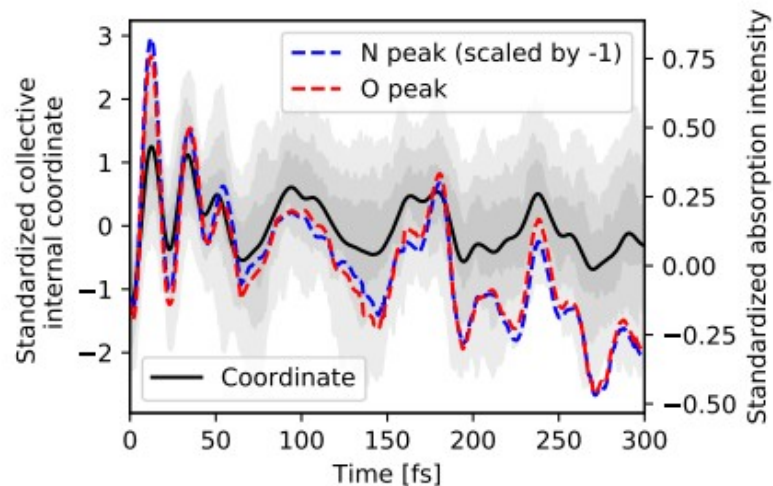
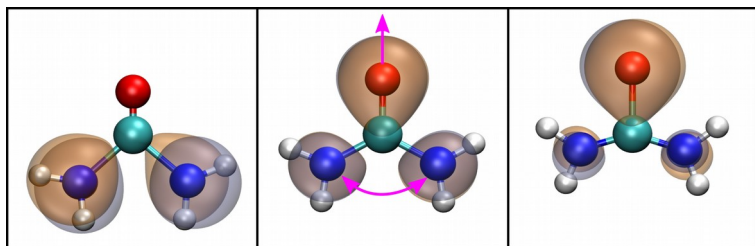
Reference

- Shakya et al., Struct. Dyn. **8**, 034102 (2021)

Thank you for listening!

Verifying collective coordinate - II

O peak: $R^2 = 77\%$



C peak: $R^2 = 30\%$

