

## Motivation and Background

- Influence of hydrocarbon reactions and diamond precipitation on internal structure and evolution of icy giant planets has been in discussion since three decades[1].
- High-pressure and high-temperature environment may facilitate chemical activity: methane dissociation to polymeric hydrocarbon chains [2], then deeper towards the core, full species separation into metallic hydrogen and carbon into diamond. [1]
- Diamond formation already obtained experimentally around 150 GPa and 5000K in polystyrene ( $C_8H_8$ ) [1] pyrolytic and polycrystalline graphite [3] at predicted H metal transition conditions.
- Nucleation driven by H – C phase separation (demixing) occurs on ns timescale.
- Confirmed diagnosis of whether H is actually turning metallic is still required.
- X-ray scattering data would help in the diagnosis of metallic H in plastic samples.

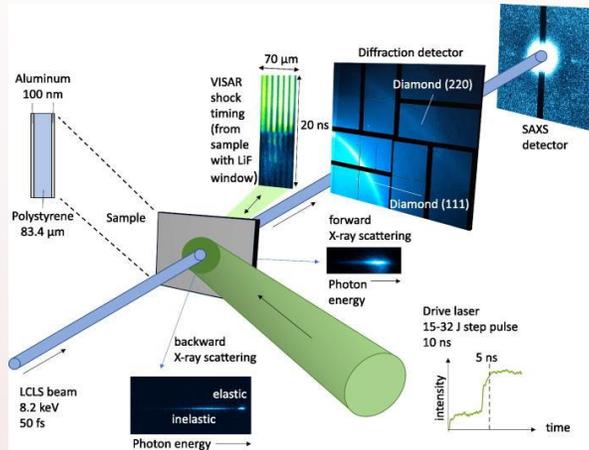


Fig 1. Experimental Setup for LCLS experiment<sup>[1]</sup>

## Method

- Computer simulations help to provide significant information before designing the experiments.
- Looked at previous data from EuXFEL experiment: no drive laser, just with x-rays, using the monochromator.

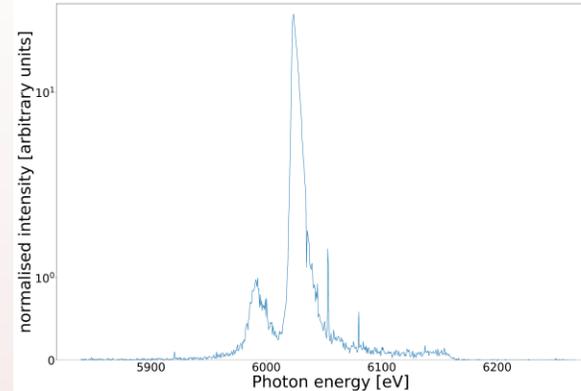


Fig 2. High-resolution forward XRTS from diamond from the EuXFEL experiment.

- Instrument function obtained: deconvolving the source spectrum from the backward scattering spectrum both in SASE mode with monochromator<sup>[4]</sup>
- Simulations were obtained for the same q-vector ( $0.94 \text{ \AA}^{-1}$ ) as in the previous EuXFEL experiment. Evaluated using the ALDA (adiabatic local density approximation) kernel for TDDFT in yambo using the Kohn-Sham orbitals evaluated using Quantum ESPRESSO. [5]
- These simulations were then convoluted with the instrument function of the experiment.

## Current Results

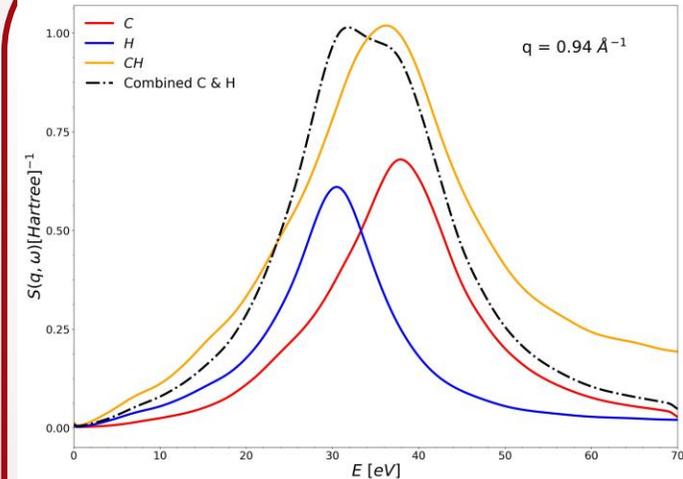


Fig 4. Comparison Graph between mixed (green) and demixed (black) C-H

- As it is already convoluted with the instrument function, we can say that we have the resolution to observe difference between fully mix CH and isolated metallic H and C together.
- If we demonstrate through experiments that we have this metallic H then it is very nice for follow ups that we can add other elements into the plastics and study chemistry of metallic H.
- Further down the line, this can not only be used for CH mixtures but also for other mixtures like H-He, for example, which would be more important for planets like Jupiter and Saturn.

## References

- [1] Kraus et al, Nat. Astron **9**, 606 (2017).  
 [2] Lobanov et al. Nat. Commun. **4**, 2446 (2013)  
 [3] Kraus et al, Nat. Commun **7**, 10970 (2016)  
 [4] Voigt et al. Physics of Plasmas **28**, 082701 (2021)  
 [5] Ramakrishna et al. J. Phys.: Condens. Matter **32** 095401 (2020)

## Acknowledgments

