QUEEN'S UNIVERSITY BELFAST

QUEEN'S UNIVERSITY IONIC LIQUID LABORATORIES QUILL

Boron Lewis Acids: A Study of Metal-Free Catalysts

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1. Background

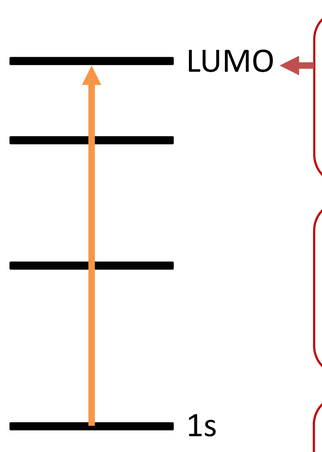
Brønsted acid – proton donor Lewis acid – electron pair acceptor

$H^+ \leftarrow :B$ $A \leftarrow :B$

Problem

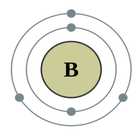
- Quantifying Lewis acidity is difficult
- Current methods rely on a probe molecule

	NMR	Computational
Hard	Gutmann-acceptor number method	Fluoride ion affinity (F^-)
Soft	Child's method	Hydride ion affinity (H^-)

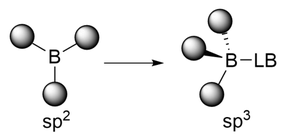


Factors that affect Lewis acidity:

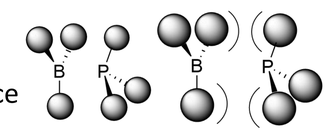
Electrotonic structure of boron centre



Energy required to change geometry



Steric hindrance



Solution

- Use X-Ray spectroscopy to isolate a component of Lewis acidity to develop a new probe-free scale

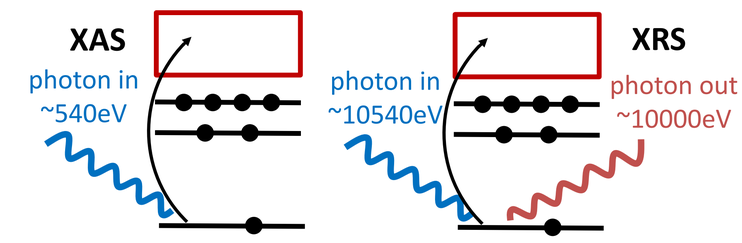
2. X-Ray Spectroscopy

X-ray Absorption Spectroscopy (XAS)

XAS tells you information about the structure however… light elements require soft x-rays and therefore a vacuum

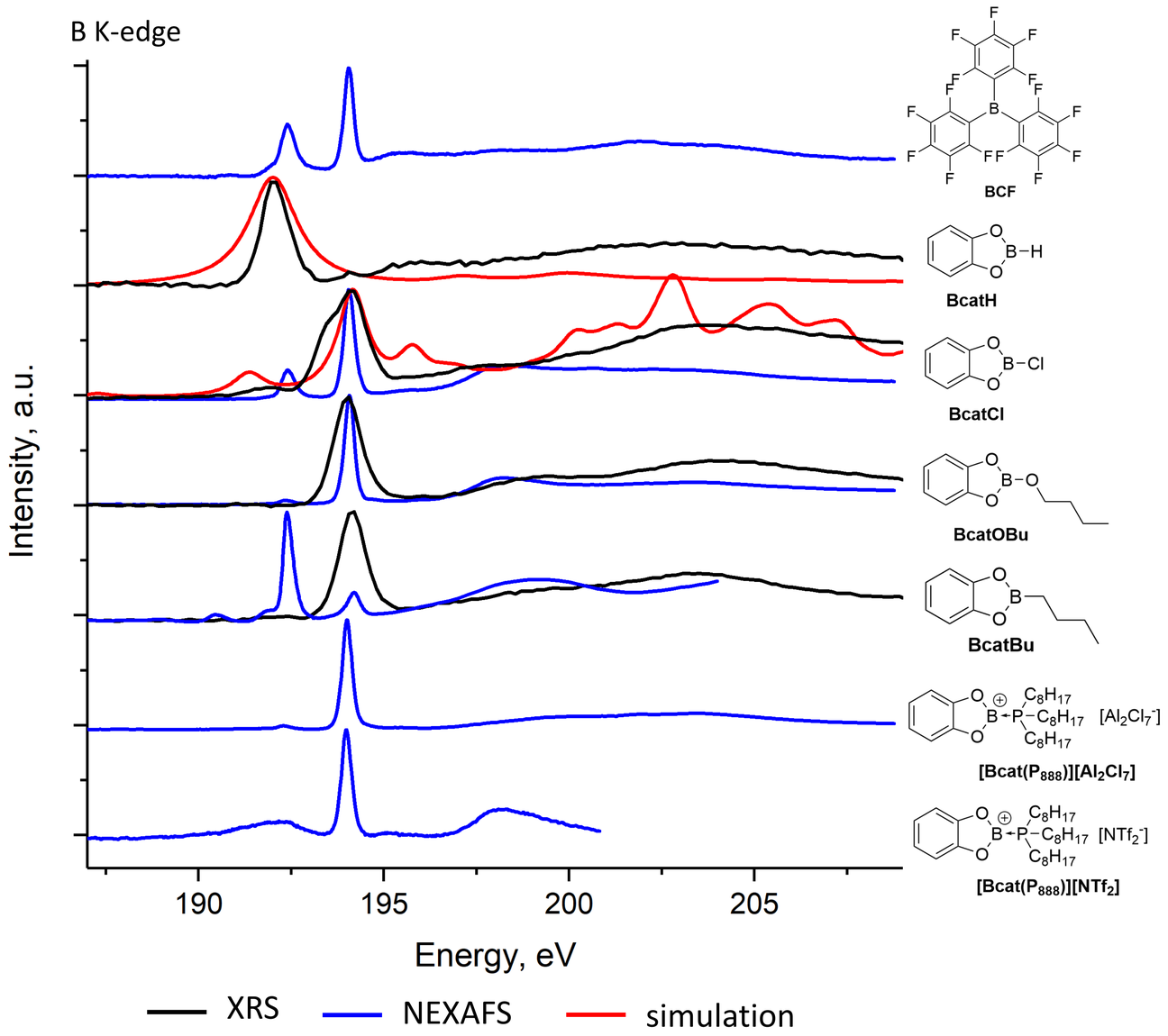
X-ray Raman Spectroscopy (XRS)

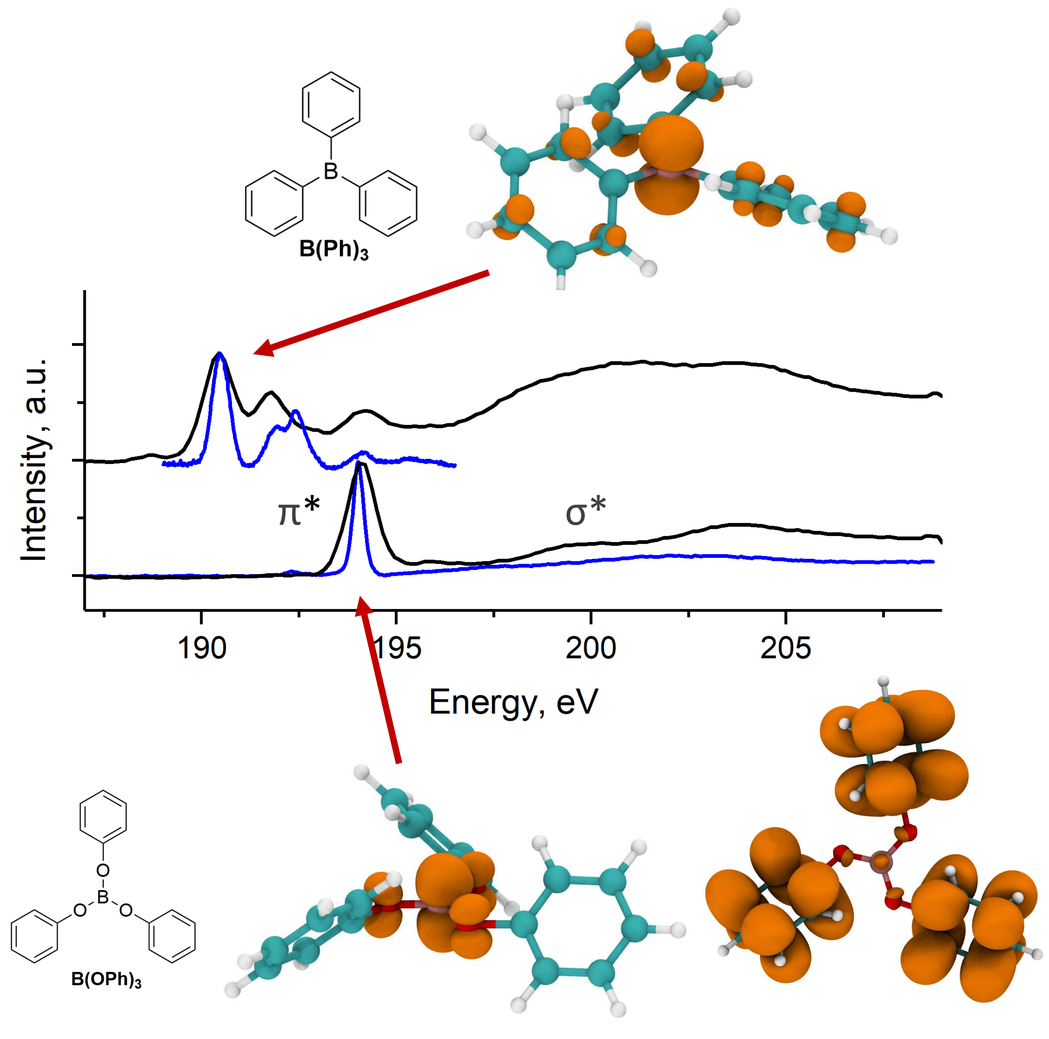
XRS is a scattering technique, using hard x-rays, enabling *operando* studies and more complex sample environments



Incident energy in XAS = energy difference in XRS

3. XRS, NEXAFS and simulation results





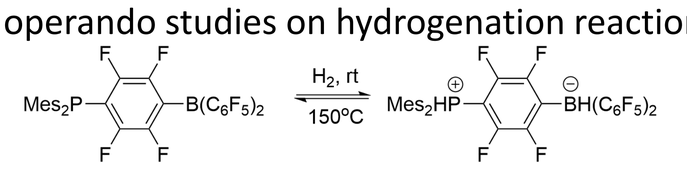
This work will drive computational models to study the electron density and therefore will be a measure of intrinsic Lewis acidity

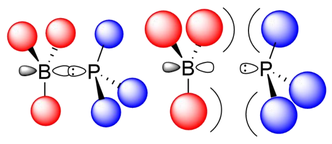
4. Conclusions

- We have measured the B K edge of a range of boron Lewis acids using soft XAS, XRS and simulations to investigate the electronic structure to correlate to electron density and relate to a component of intrinsic Lewis acidity.

5. Future work

- Combine this work with experimentally driven computational models to derive a measure of intrinsic Lewis acidity from the electron density
- Additionally, combine these boron Lewis acids with a base in a Frustrated Lewis pair (FLP).
- Eventually conduct operando studies on hydrogenation reactions with FLP-SILP systems.





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