Lessons from the beamline:
The TES detector at beamline 10-1

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Kelsey Morgan
Galen O’Neil
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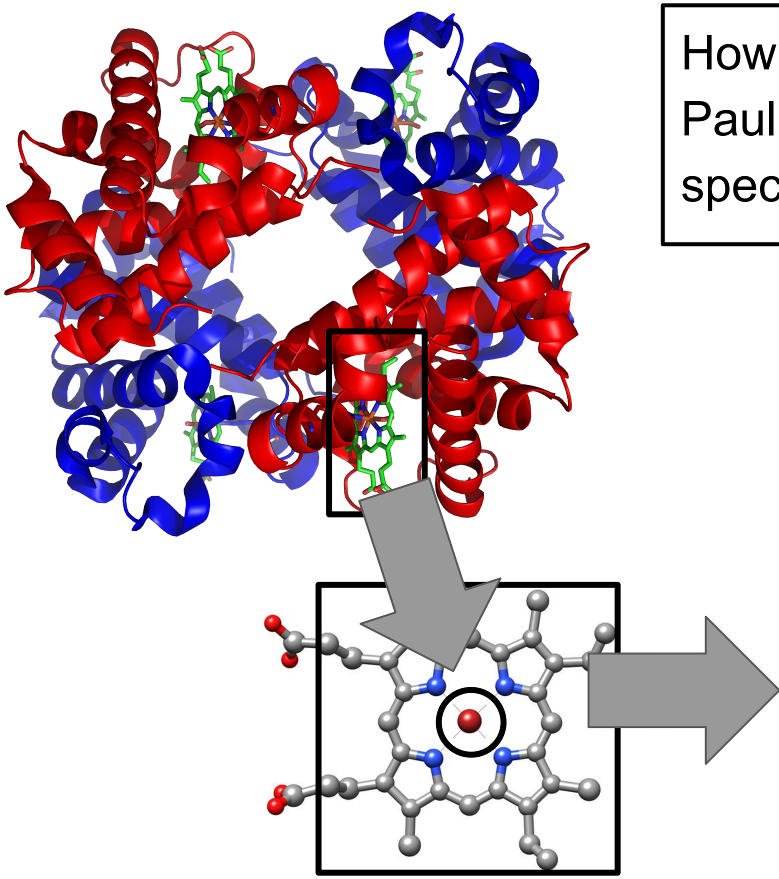
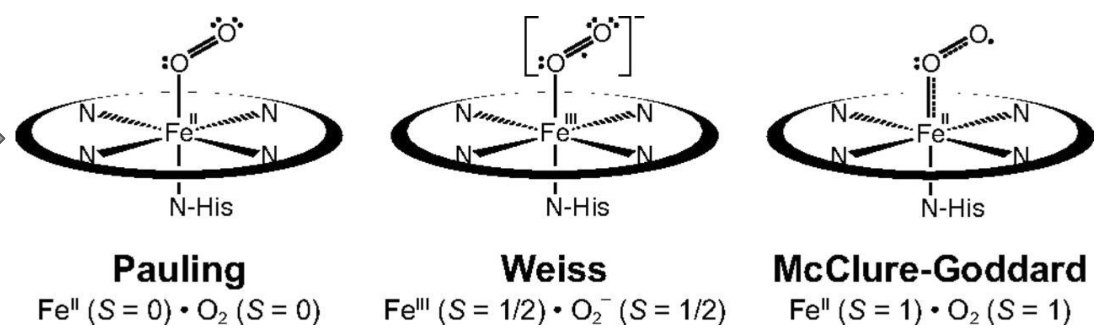
Daniel Schmidt
Daniel Swetz
Joel Ullom

How does hemoglobin transport oxygen?



How does iron bind to oxygen in hemoglobin? Pauling's first model published in **1936**. Can X-ray spectroscopy solve this **80-year old mystery**?

Controversy: whose model is best?

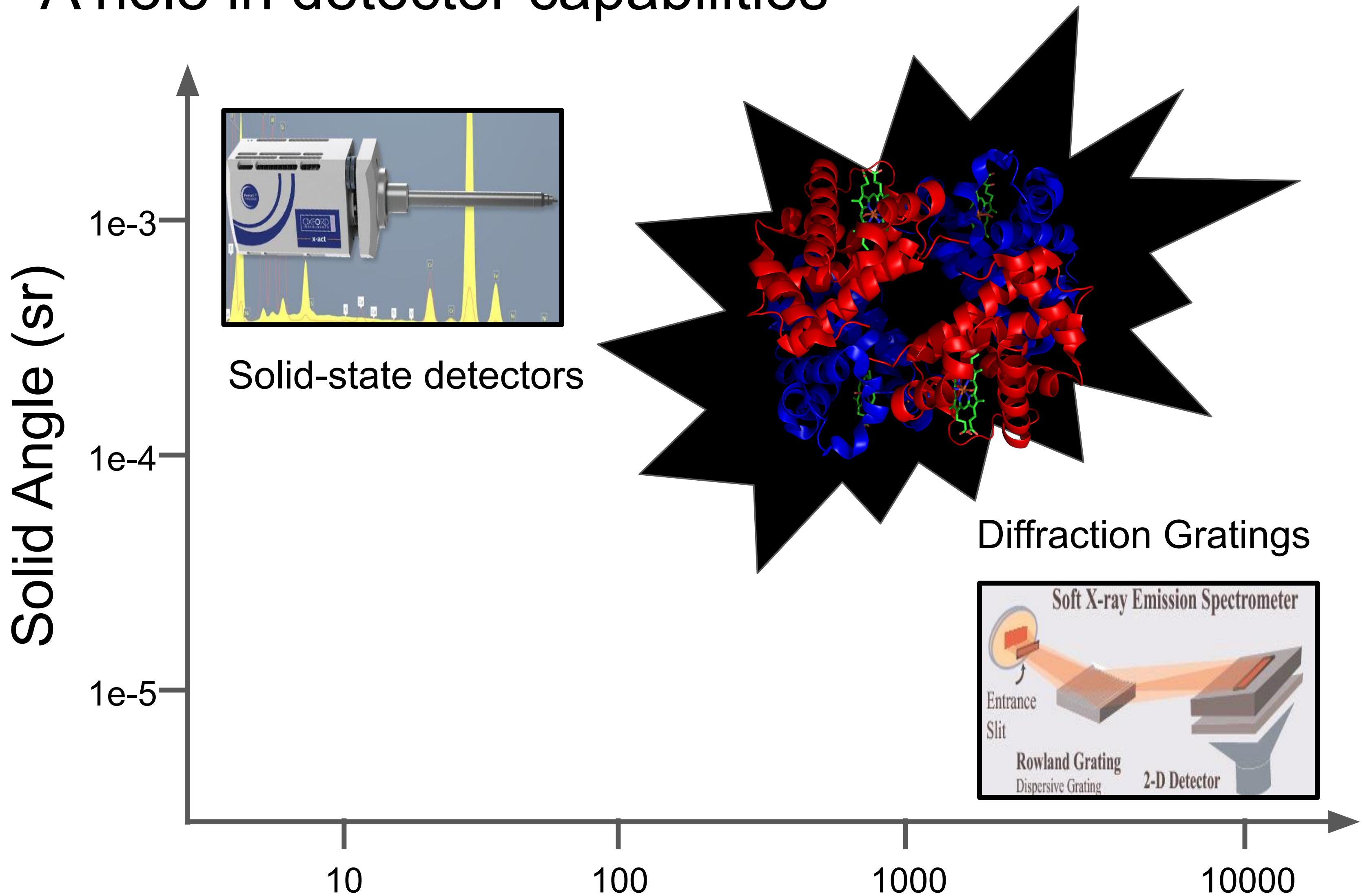


Wilson, S. A., et al (2013). *PNAS*, *110*(41)

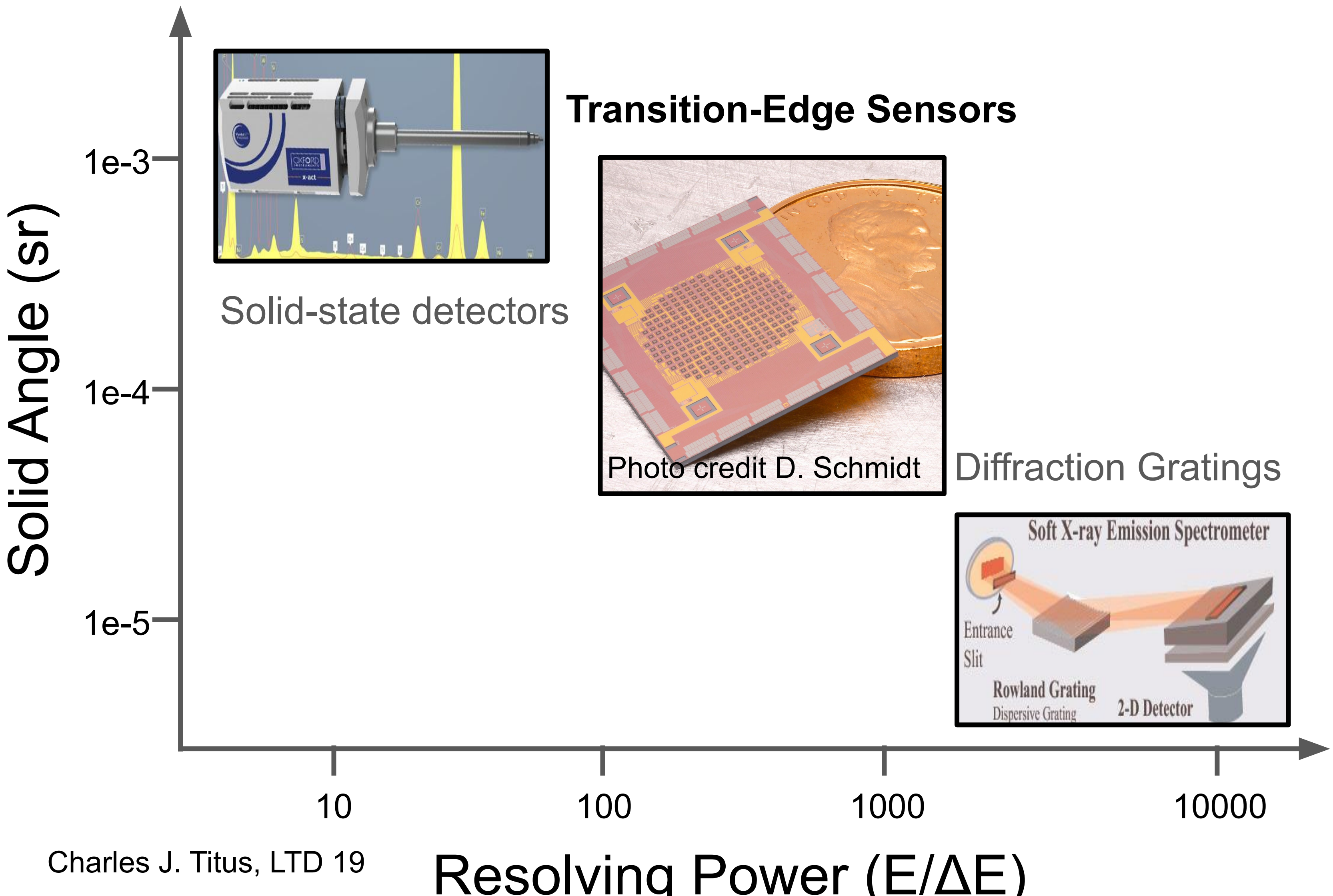
Outline

- **The TES advantage**
- Science at SSRL using a TES
  - Understanding battery degradation
  - Detecting contaminants in carbon nanotubes
  - Measuring the Fe-O bond in hemoglobin

A hole in detector capabilities



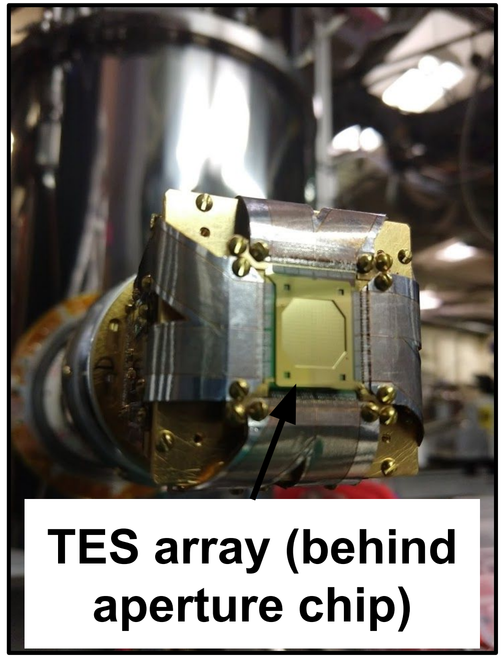
Can be filled by TES detectors!

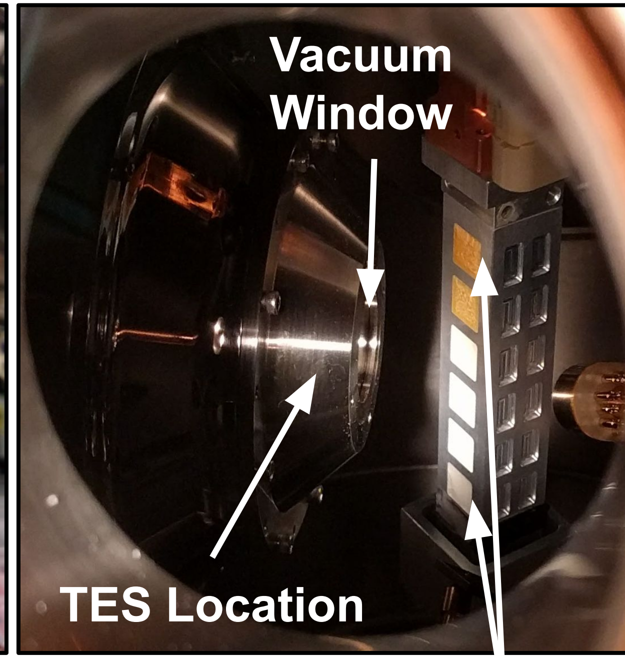


TES at SSRL BL 10-1 available for users since 2017

Array Specs

Pixels	240
Solid Angle	2e-3 sr
Energy range	200-2000 eV



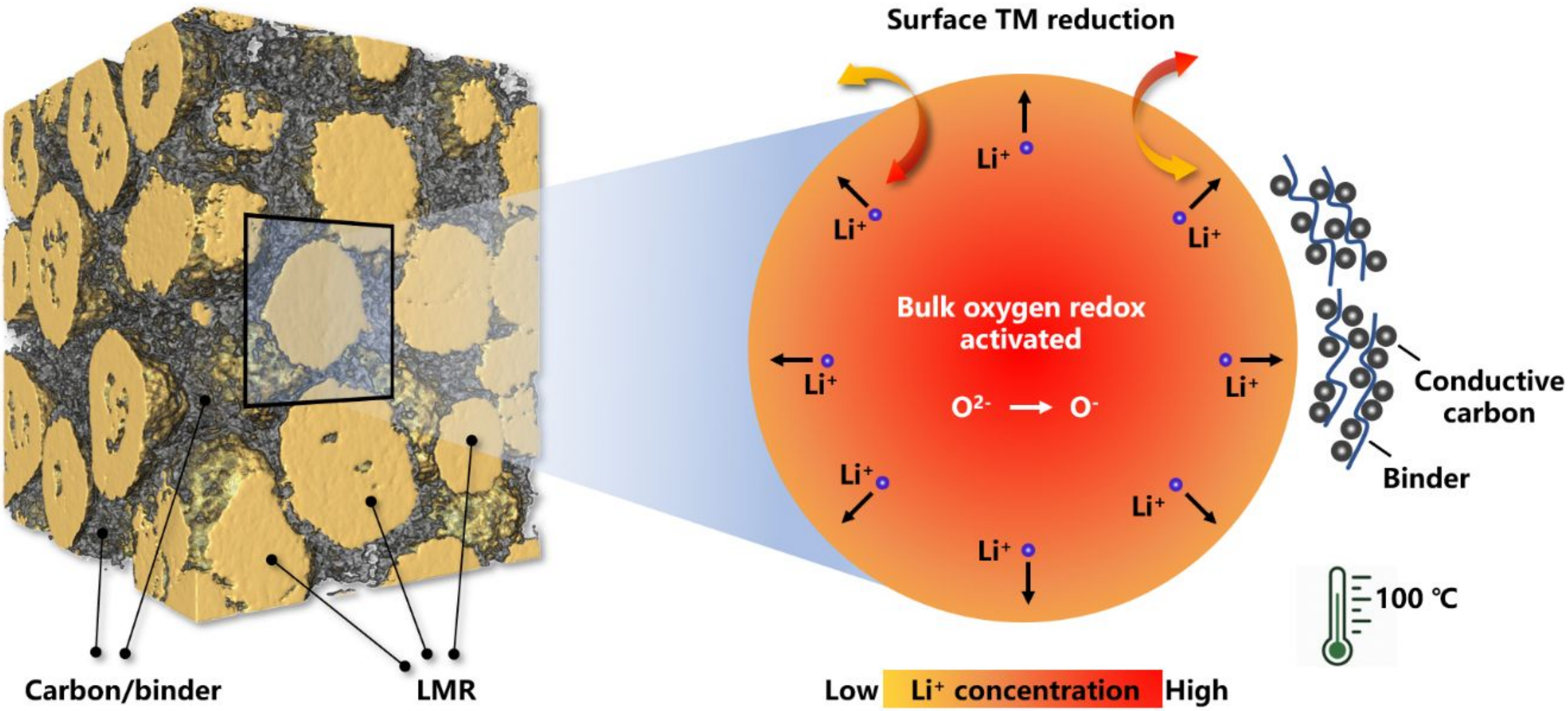


Pixel Specs

Mo/Cu bilayer thickness	60 nm/200 nm
Tc	107 mK
Energy Resolution	1.5 eV @ 500 eV
Absorber thickness	2.8 um Bi

System details in
Doriese, et al (2017). Rev. Sci. Instrum., 88(5), 53108.

What causes thermal degradation of batteries?



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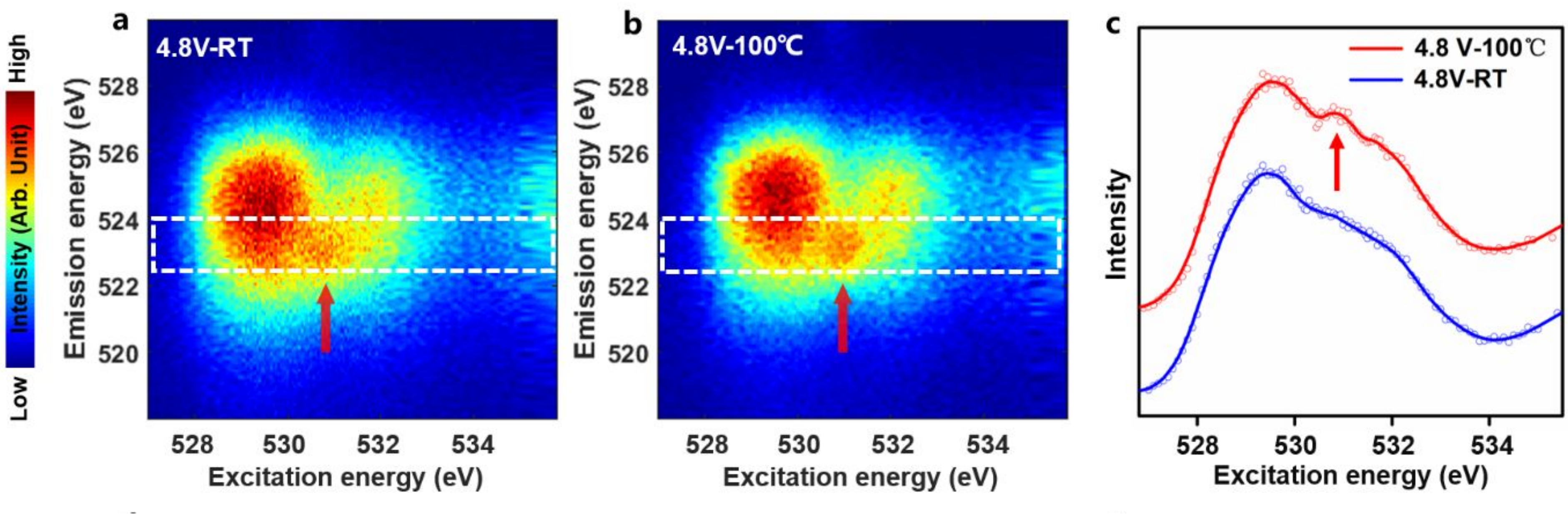
Li et al, *J. Am .Chem. Soc.* 2019 (Accepted)

TES reveals that oxidation is the culprit

- Small changes in oxygen spectra indicate oxidation
- This work possible at SSRL for the first time, due to TES

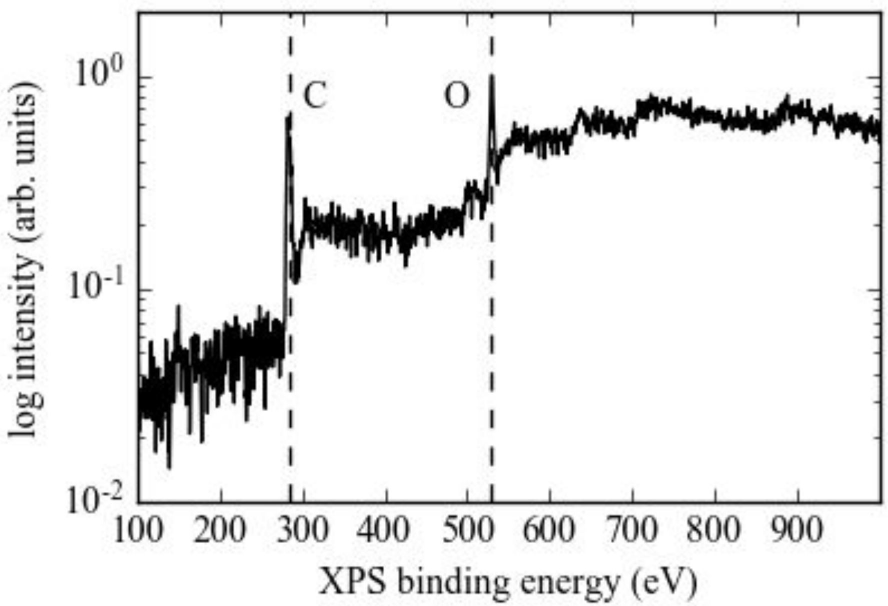


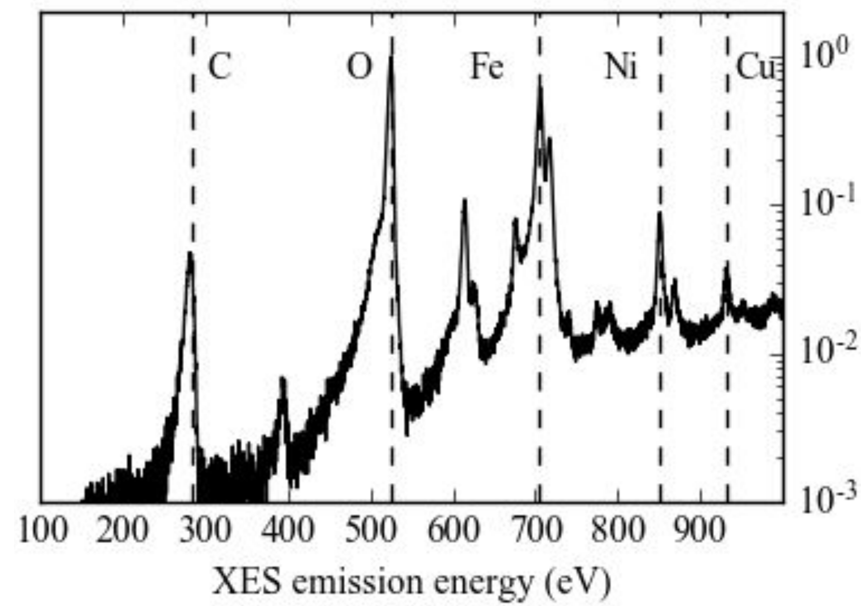
Li et al, *J. Am .Chem. Soc.* 2019 (Accepted)

What is contaminating carbon nanotube devices?

- TES shows a bunch of weird metals!
- Contaminants (<0.1%) affect device function
- TES more sensitive than other common probes (XPS)

XPS Composition Analysis vs TES Composition Analysis



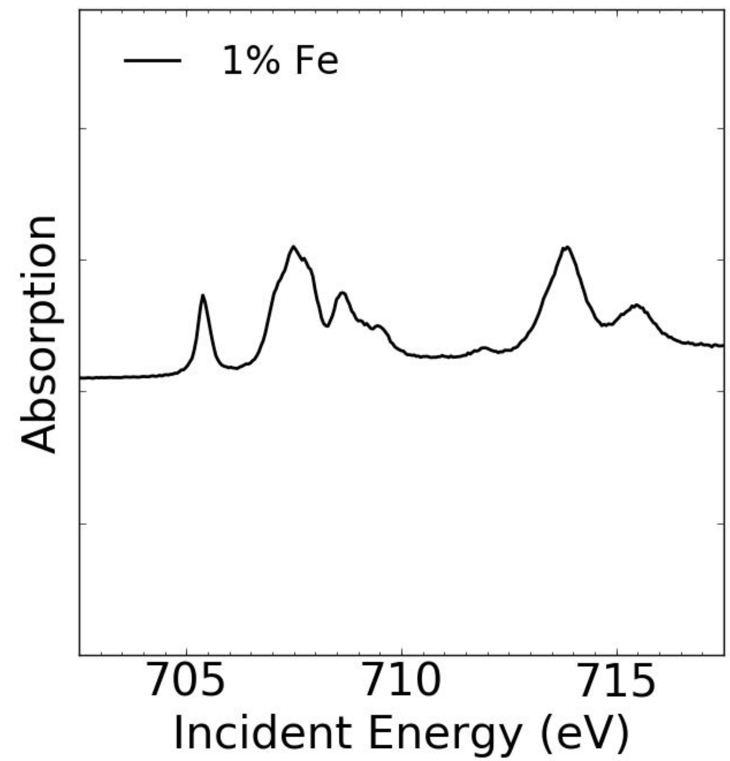


Sainio et al, *J. Phys. Chem. C*, 123, 10 (2019)

How well can we measure ultra-dilute samples?

Atomic %	Examples
>1% (concentrated)	Batteries, molecules, bulk solids

XAS of diluted $Fe(CN)_6$



Titus et al, *J. Chem. Phys.* 147, 214201 (2017)

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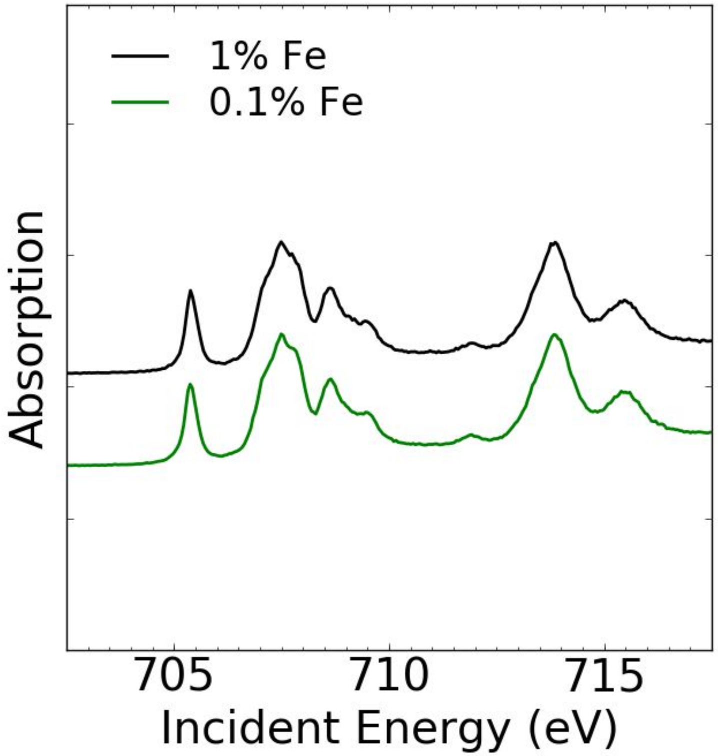

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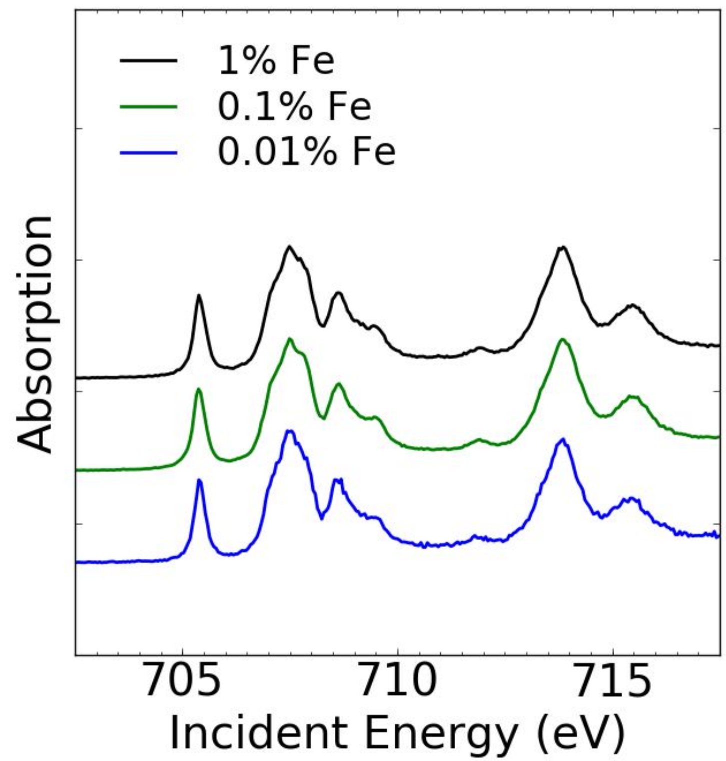


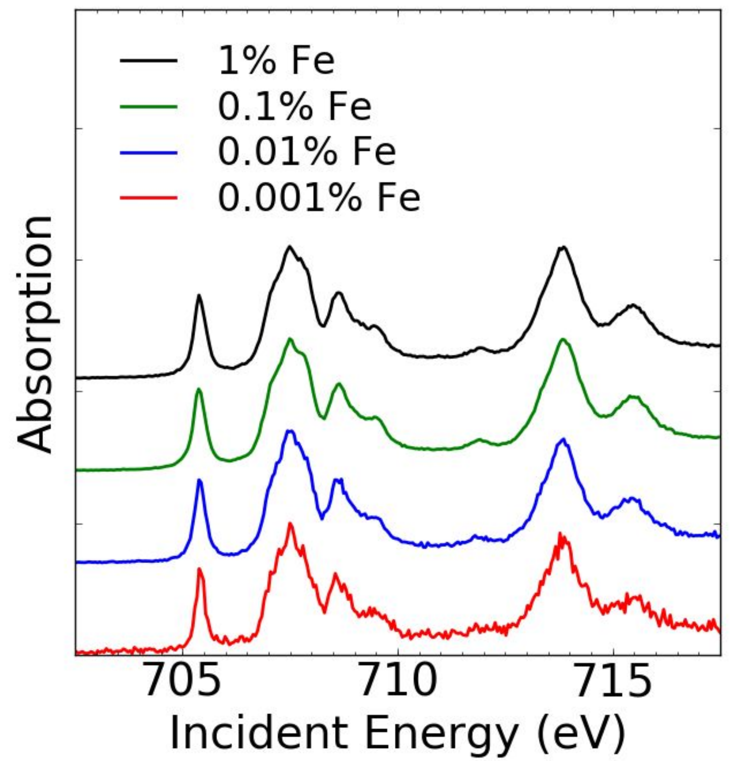
Titus et al, *J. Chem. Phys.* 147, 214201 (2017)

Excellent measurements of ultra-dilute samples

Atomic %	Examples
>1% (concentrated)	Batteries, molecules, bulk solids
0.1% (dilute)	Contaminants, solutions
0.01% (very dilute)	Hemoglobin, many proteins, monolayers
0.001% (ultra-dilute)	Photosystem-II, doped monolayers, trace impurities, color centers

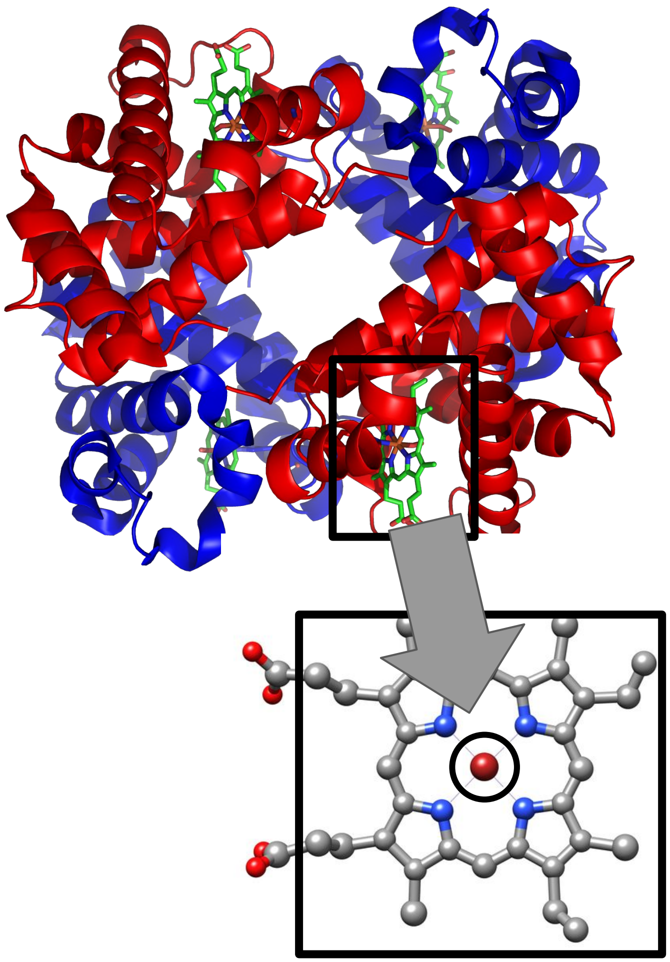
New capability: 0.001% measurement opens many doors!

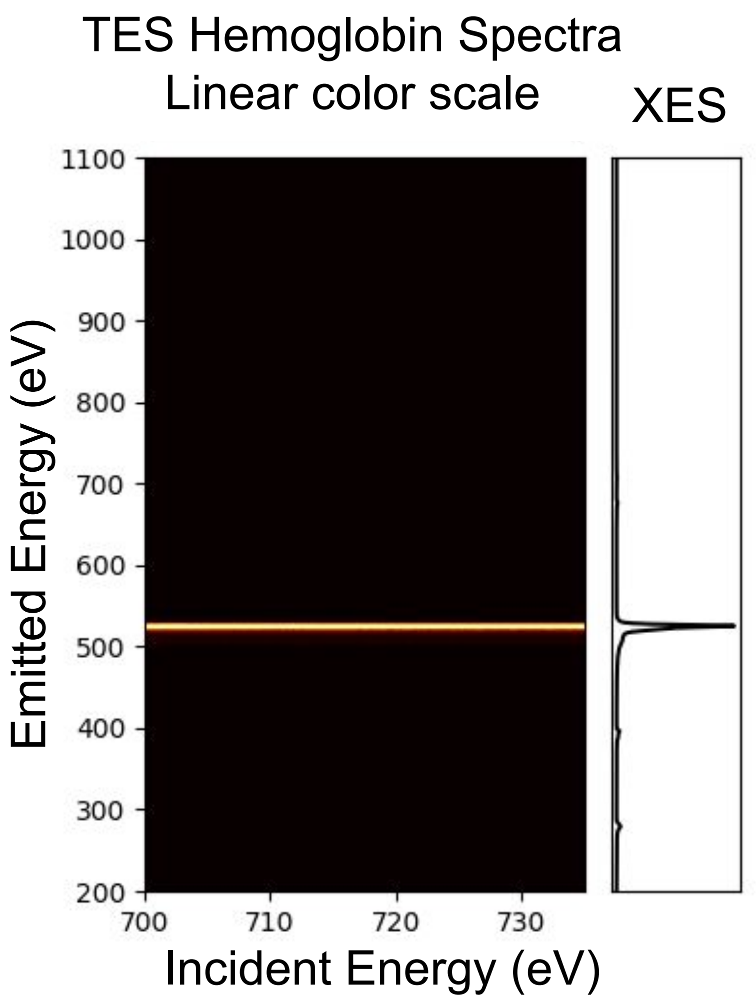
XAS of diluted $Fe(CN)_6$



Titus et al, *J. Chem. Phys.* 147, 214201 (2017)

So can we measure hemoglobin?



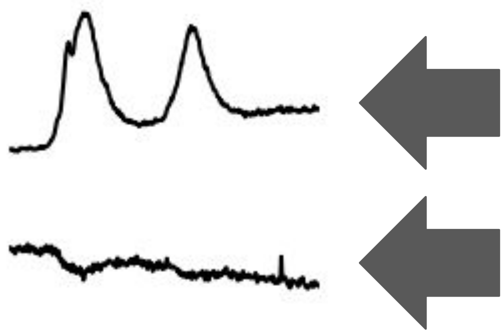


Yes!

TES has the sensitivity to reveal the Fe L-edge of hemoglobin for the first time

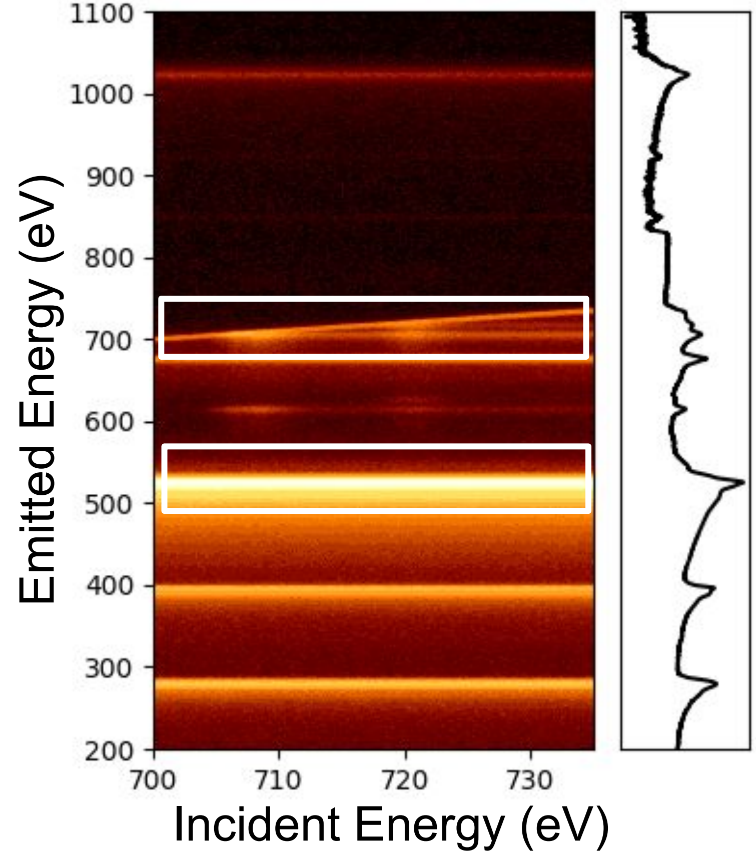
Signal!

Background!

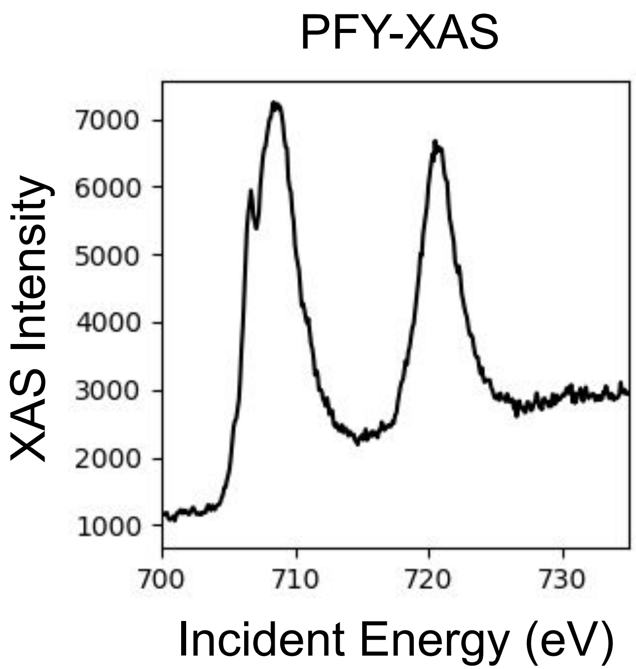


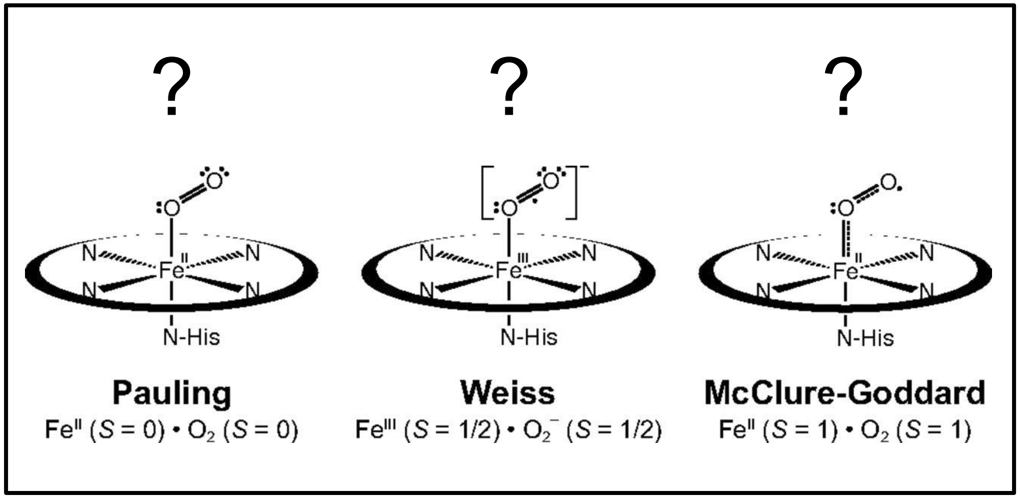
TES Hemoglobin Spectra
Log color scale

XES



First soft X-ray spectrum for oxyhemoglobin





Who is right? Analysis is ongoing!

Hemoglobin project in collaboration with:

Stanford University
Leland Gee
Augustus Braun
James Yan
Ed Solomon

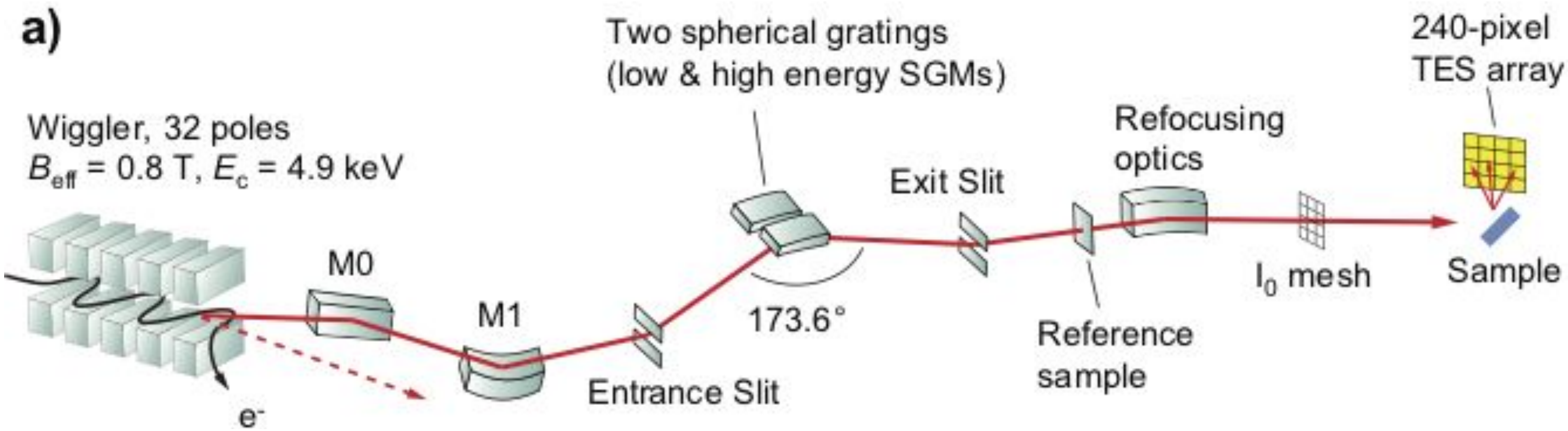
University of Manchester
Michael Baker

Conclusions

- Robust beamline instrument with strong user demand
- TES enables battery measurements previously impossible at older light-sources
- A fast, non-destructive probe of composition
- TES enables new science in dilute compounds

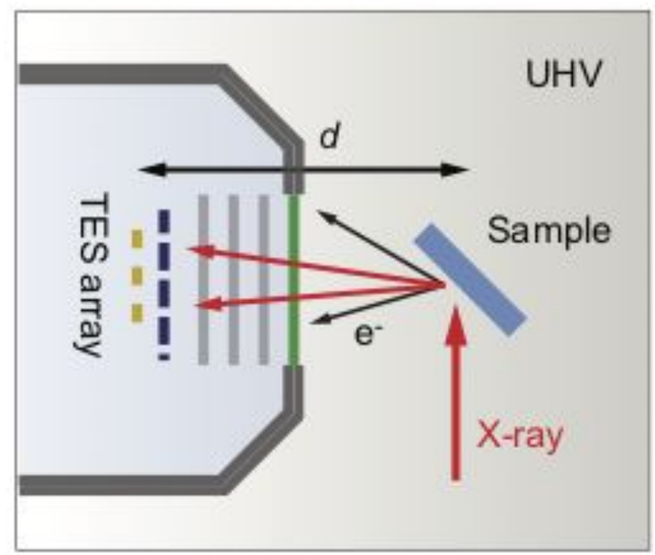
Extra Slides

TES at SSRL BL 10-1



Beamline 10-1 parameters

Photon Flux	~10^{11} phot/s
Energy Range	150-1400 eV
TES-sample distance	40 mm
Vacuum	10^{-8} torr



Soft X-ray Spectroscopy (150 eV - 1500 eV)

Element-specific probe of:

- Chemical composition
- Electronic structure
- Spin
- Symmetry

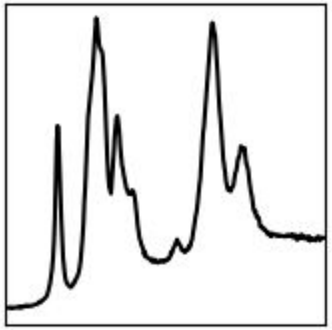
L-edges (2p)

Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn

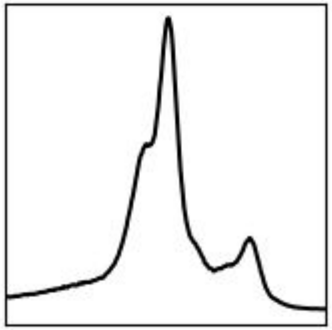
K-edge (1s)

B	C	N	O	F

Absorption



Emission

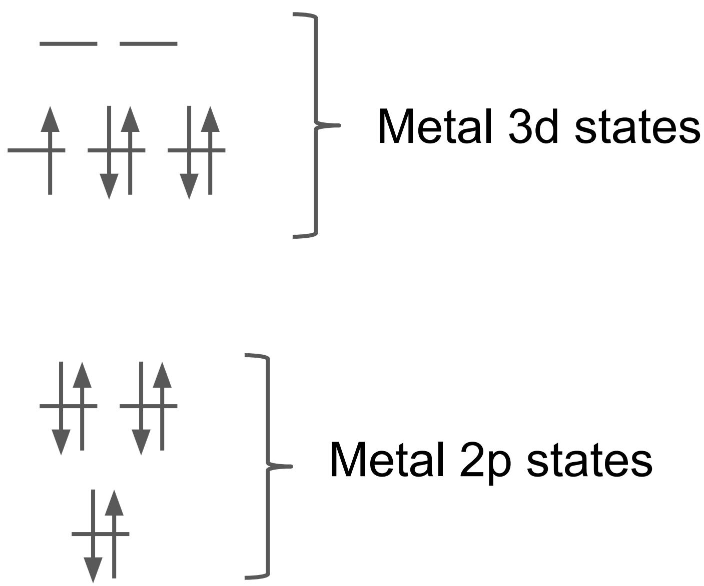


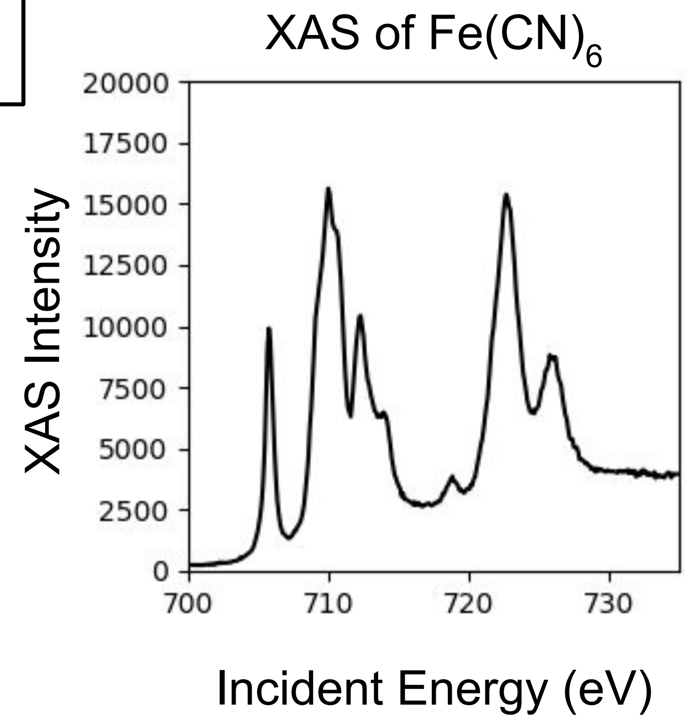
Resonant Scattering

Charles

X-ray Absorption Spectroscopy (XAS)

A photon is absorbed and kicks an electron to a higher energy level





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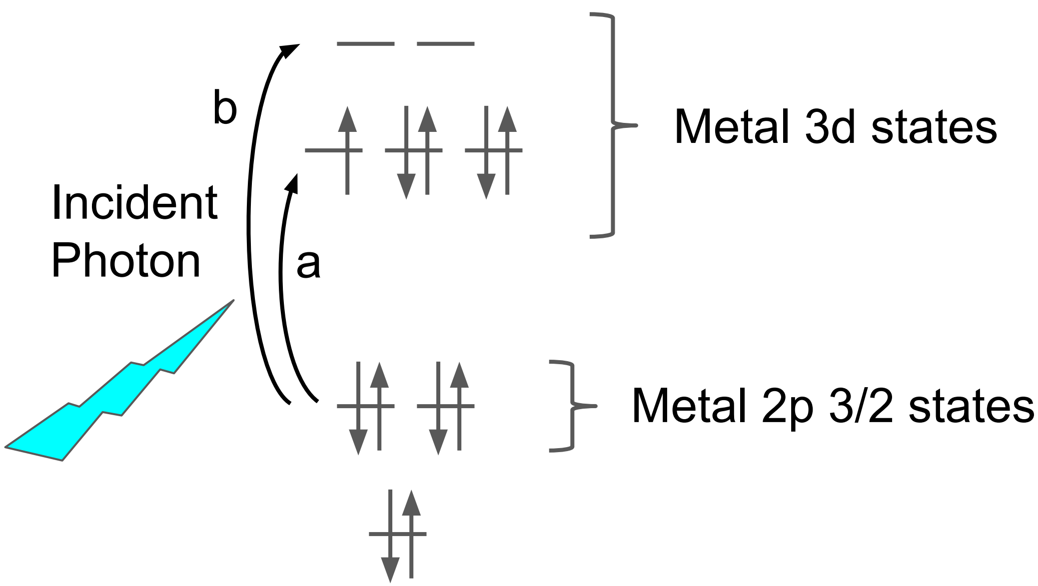

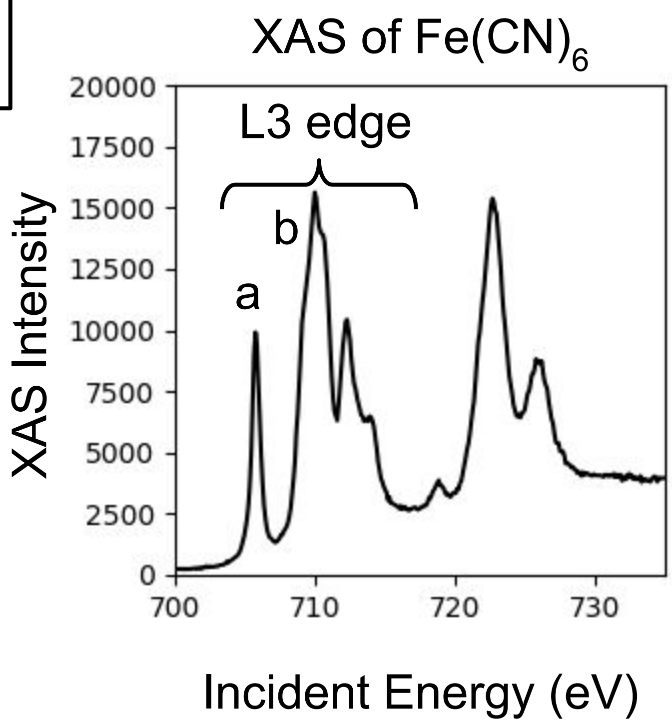

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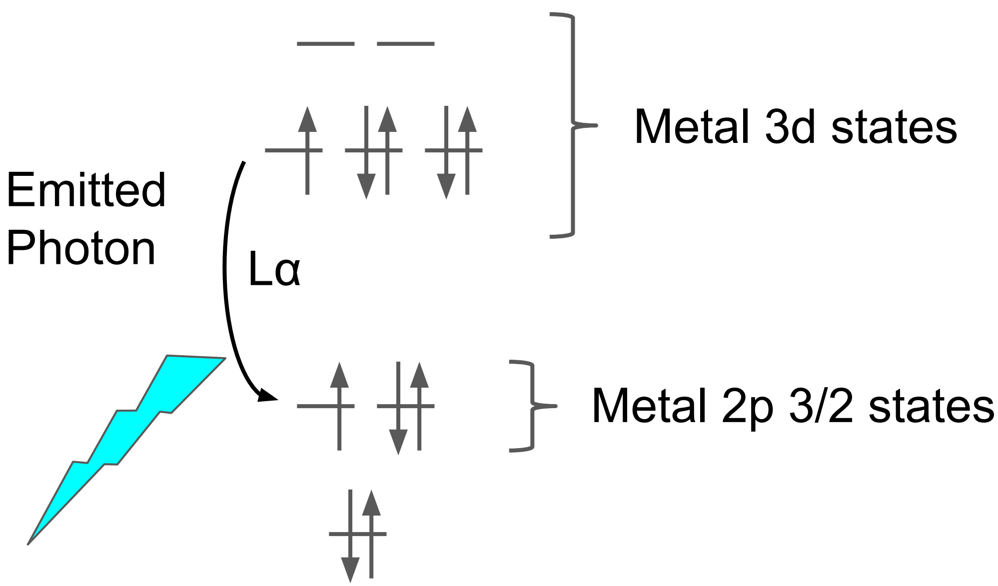
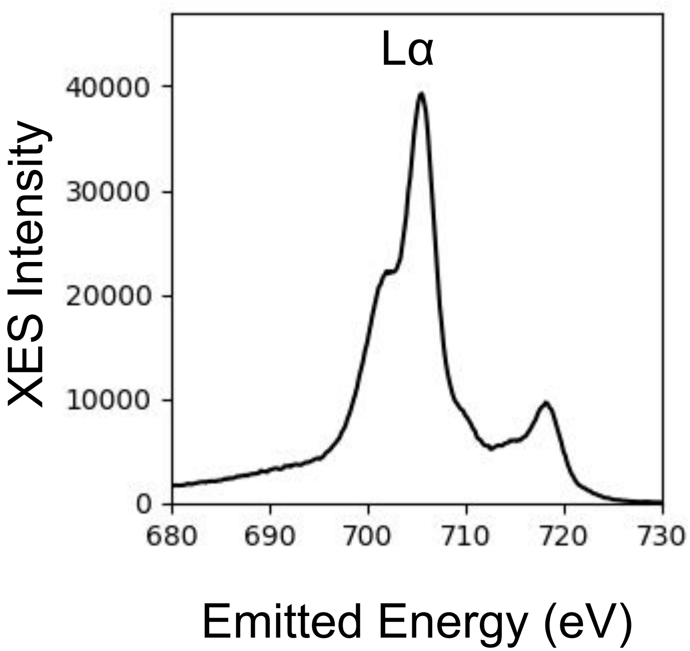
X-ray Emission Spectroscopy (XES)

A photon is emitted when an electron fills a core hole



XES of $Fe(CN)_6$



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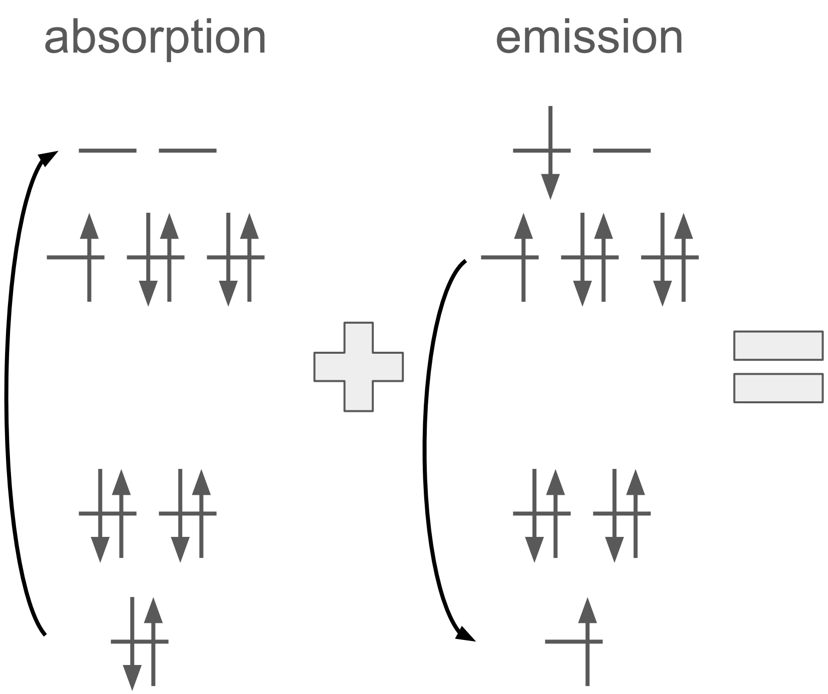
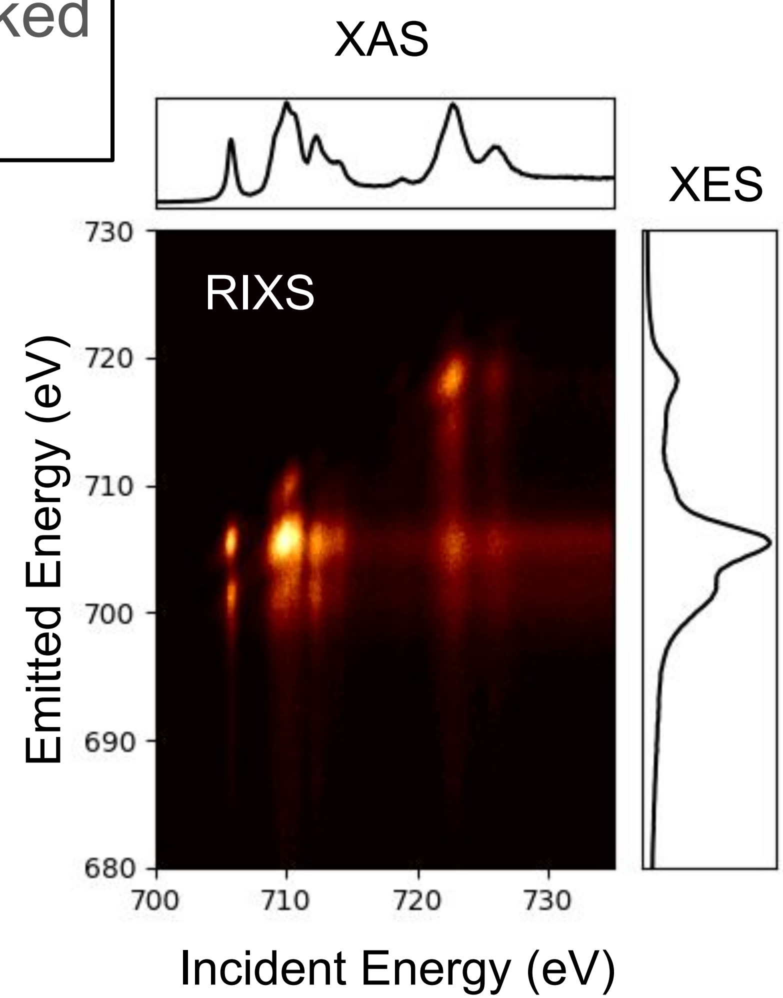
Resonant Inelastic X-ray Spectroscopy (RIXS)

Absorption and emission are linked together in a resonant process





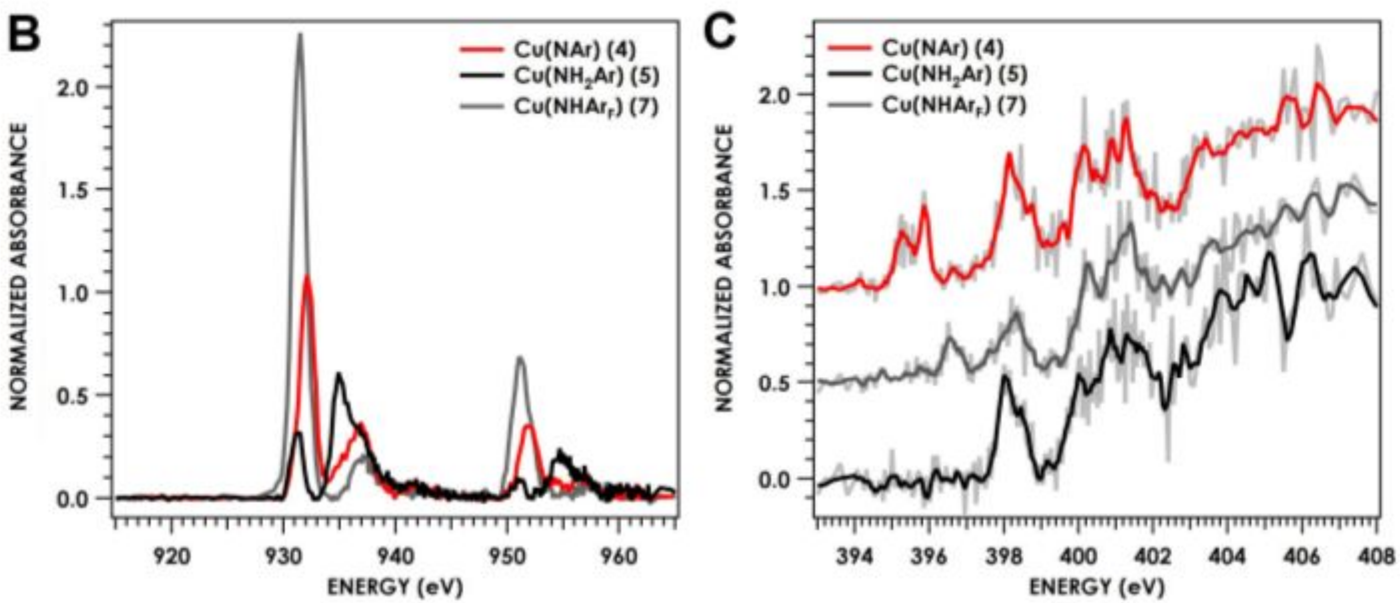
Routine Spectroscopy

Requirements

- Moderate solid angle
- Moderate energy resolution

Applications

- Everything



Carsch et al, 2019 (In revision)