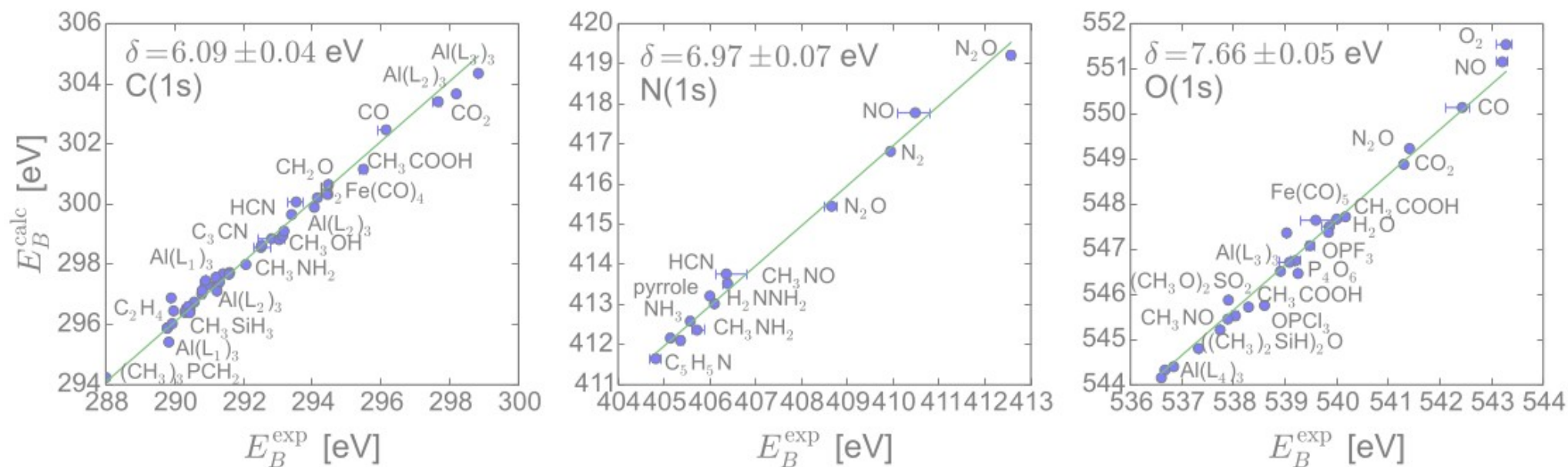


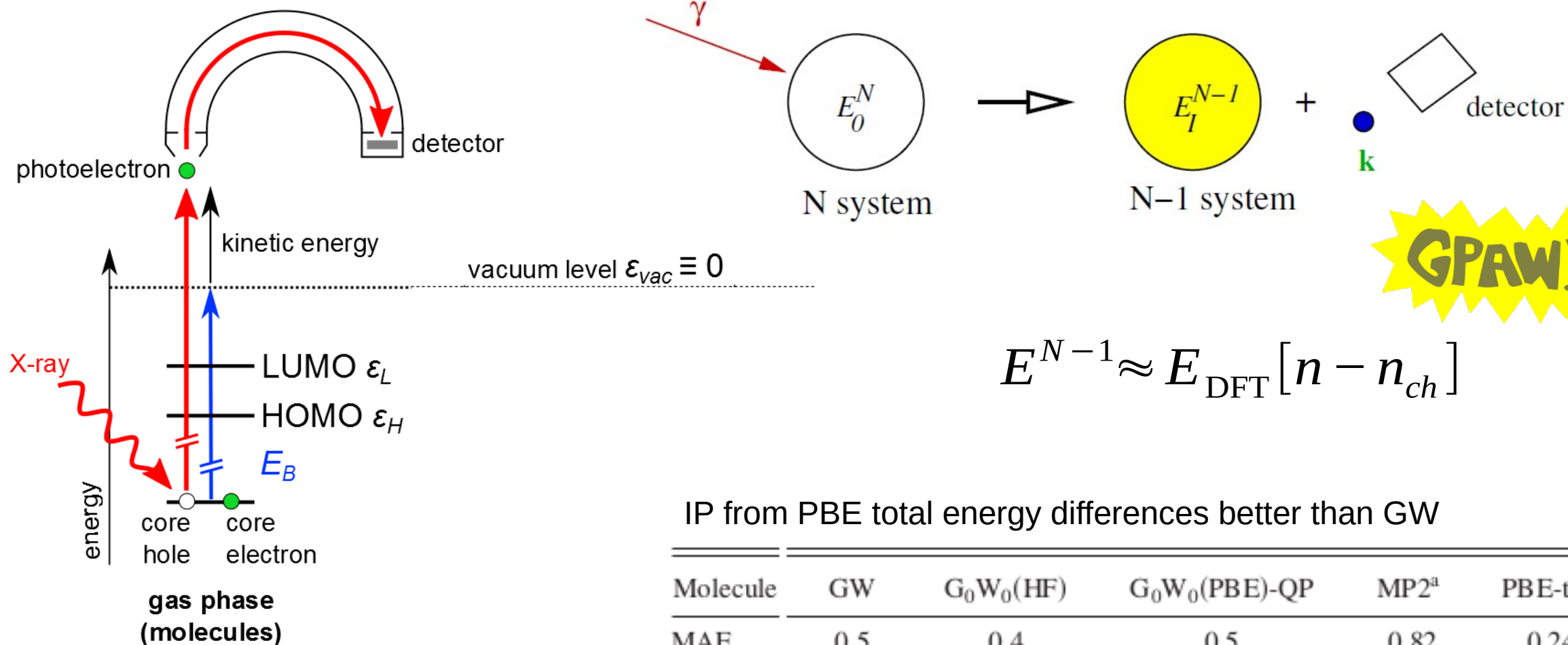
Predicting x-ray absorption and photoemission spectra on the absolute energy scale

Michael Walter, Sunel de Kock, Michael Moseler, Lars Pastewka





Molecular gas-phase XPS – energy consideration

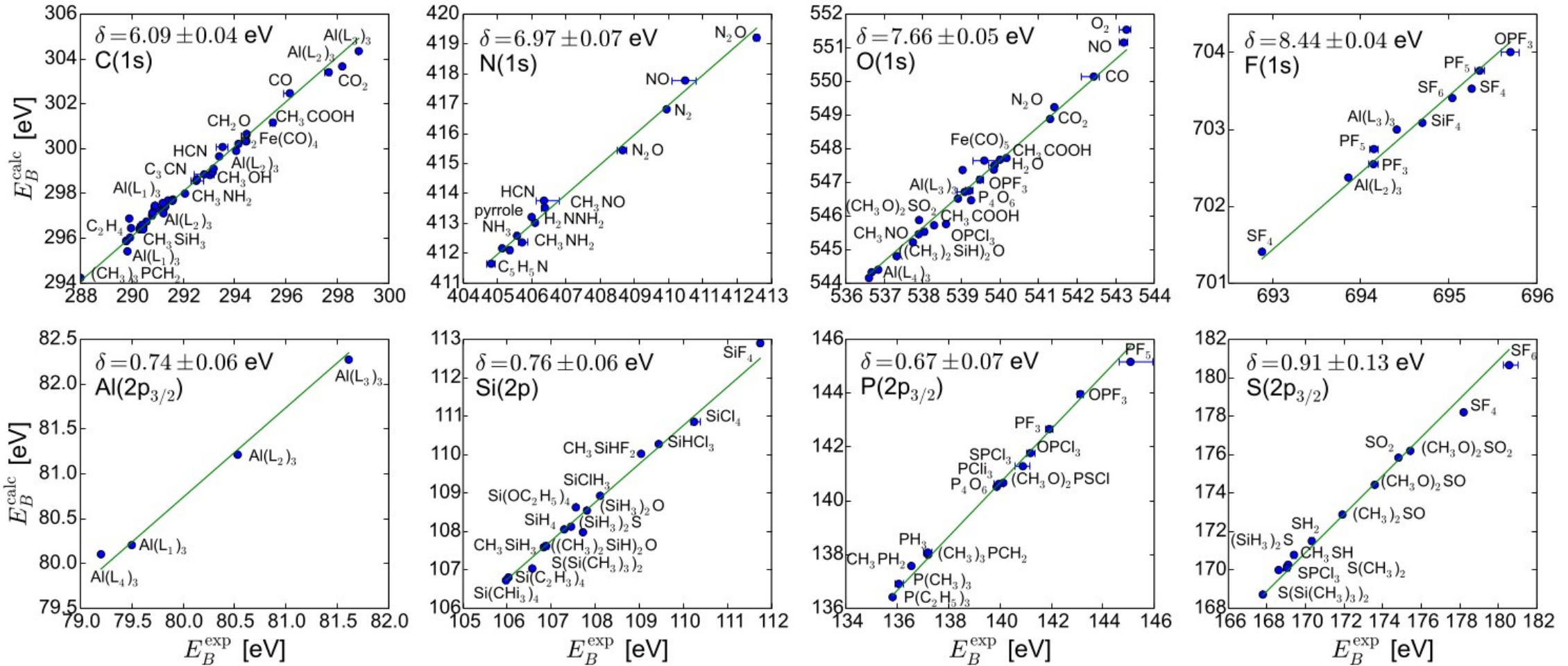


MW, Moseler, Pastewka *PRB* **94** (2016) 041112(R)

Rostgaard, Jacobsen, Thygensen *PRB* **81** (2010) 085103



Molecular gas-phase XPS spectra

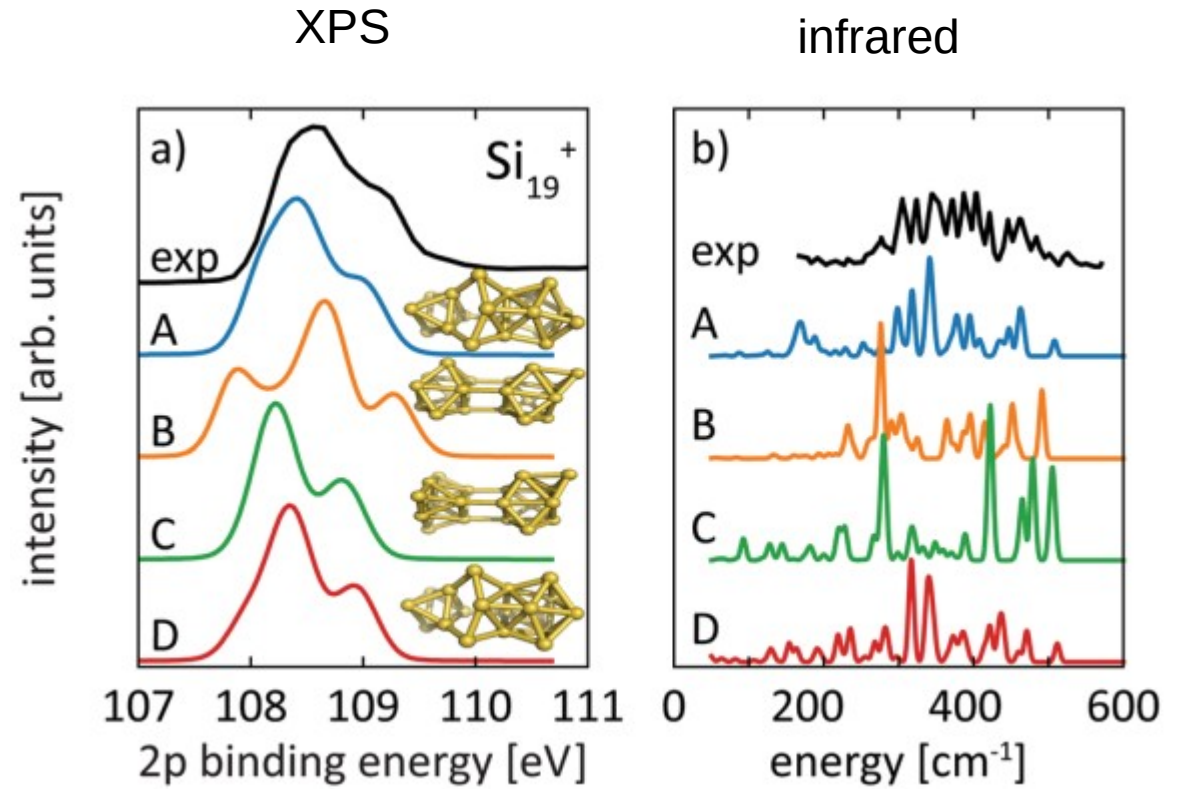
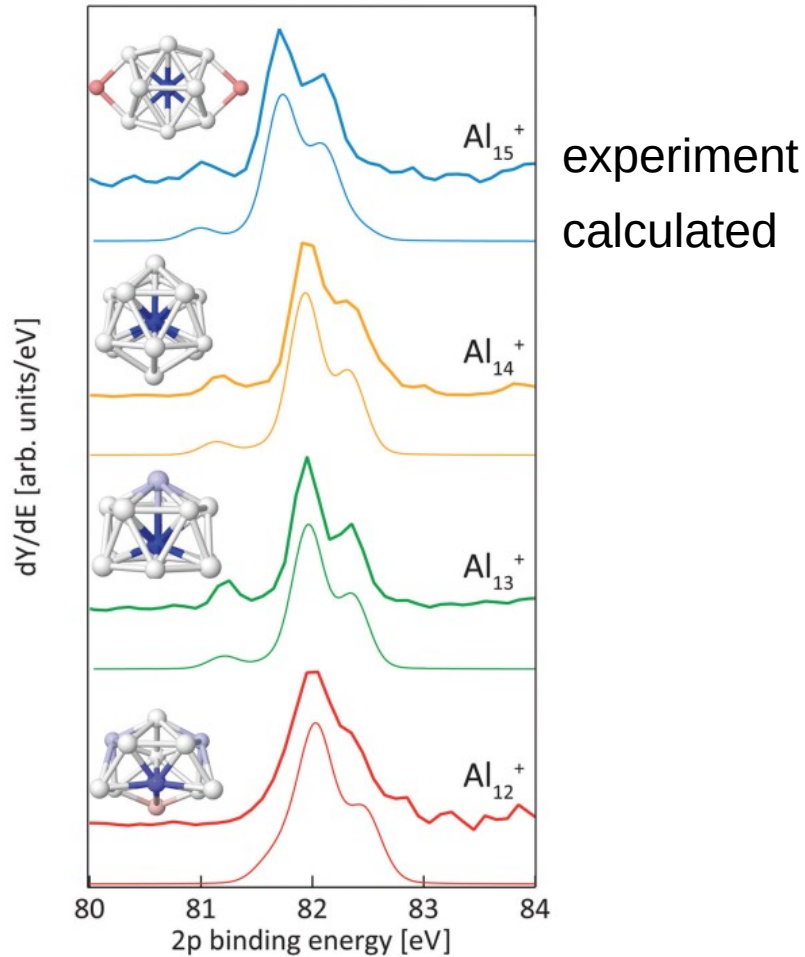


MW, Moseler, Pastewka PRB 94 (2016) 041112(R)

=> empirical shift (corehole state, xc)



Application: structure determination in clusters

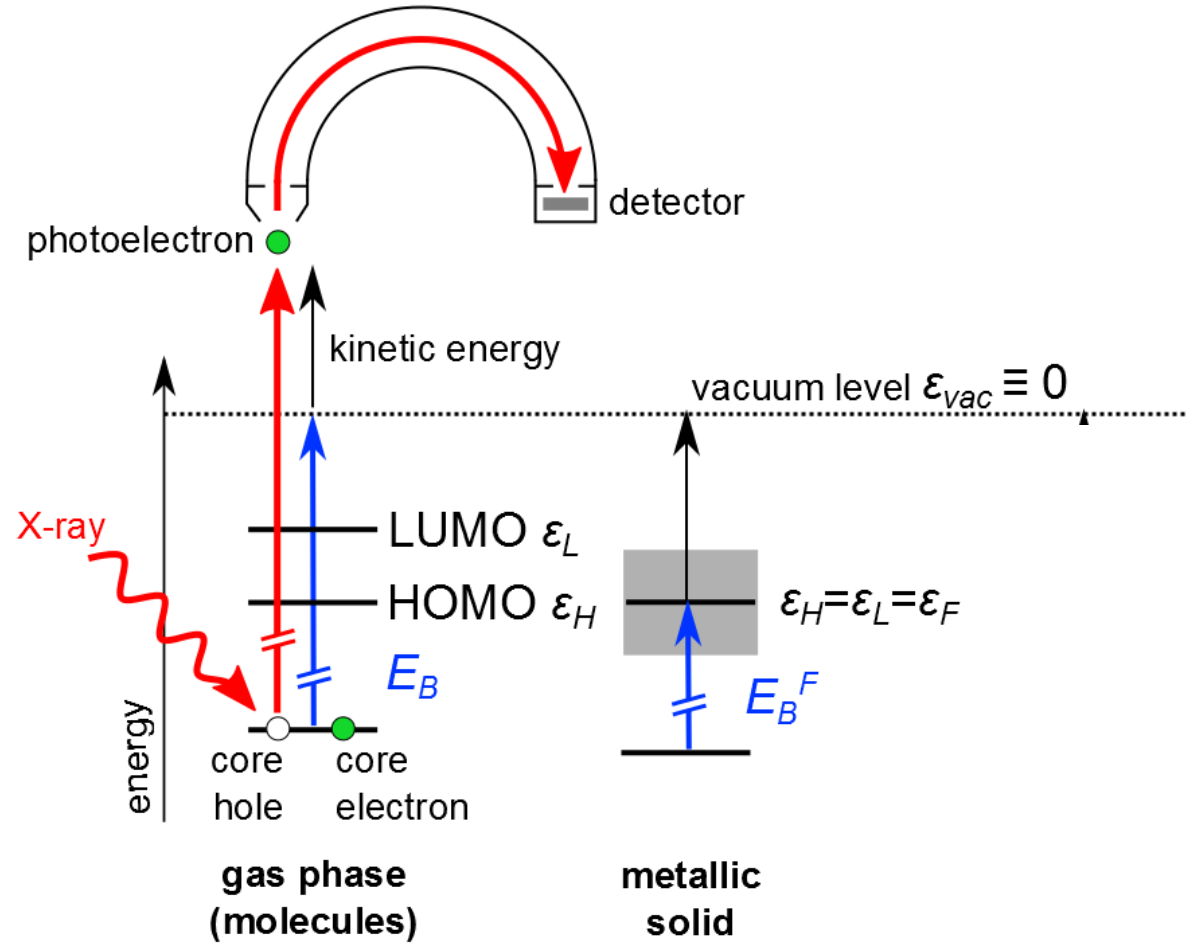


MW et al PCCP 21 (2019) 6651

=> XPS structure sensitive



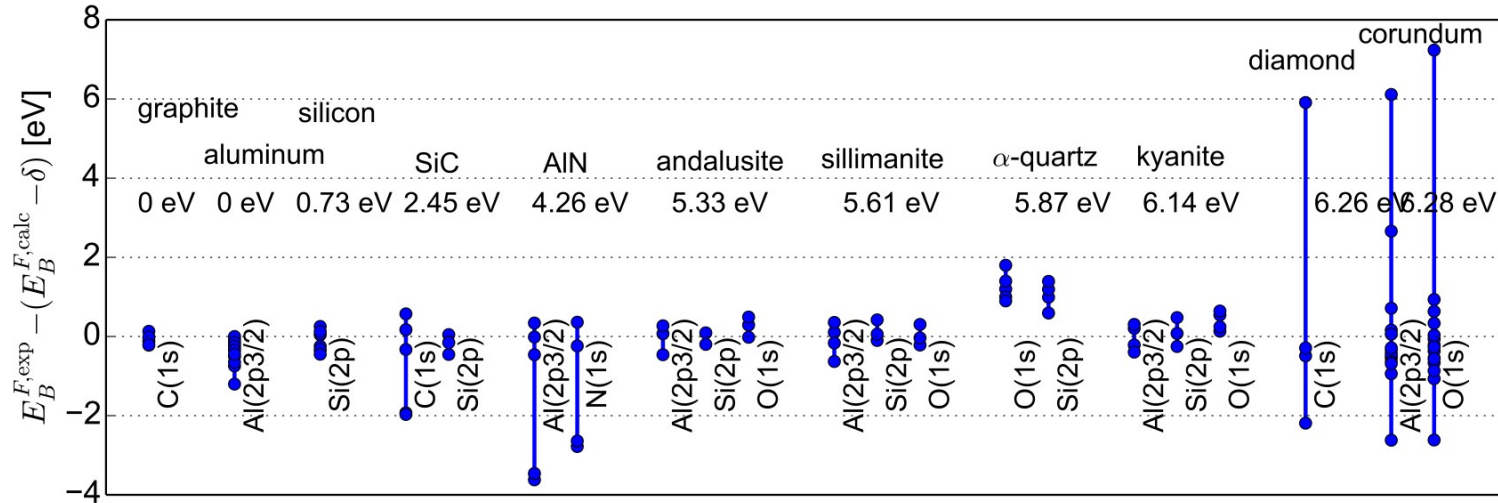
XPS spectra in solids



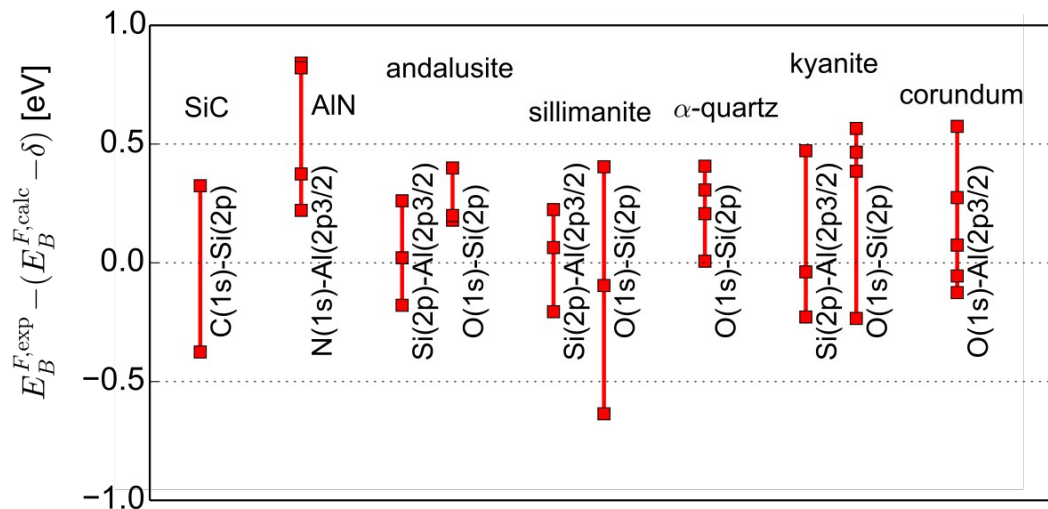
MW, Moseler, Pastewka *PRB* **94** (2016) 041112(R)



XPS spectra in solids



large variation
through large gap

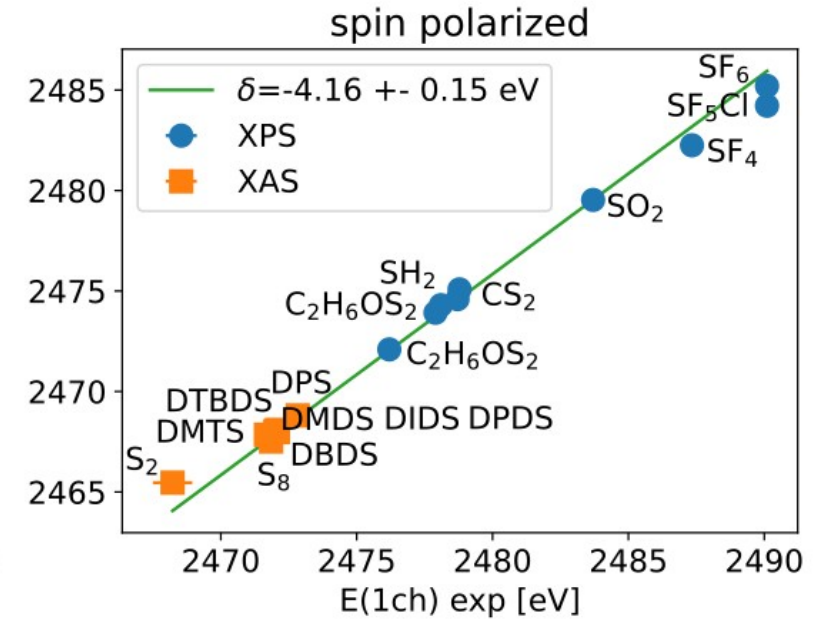
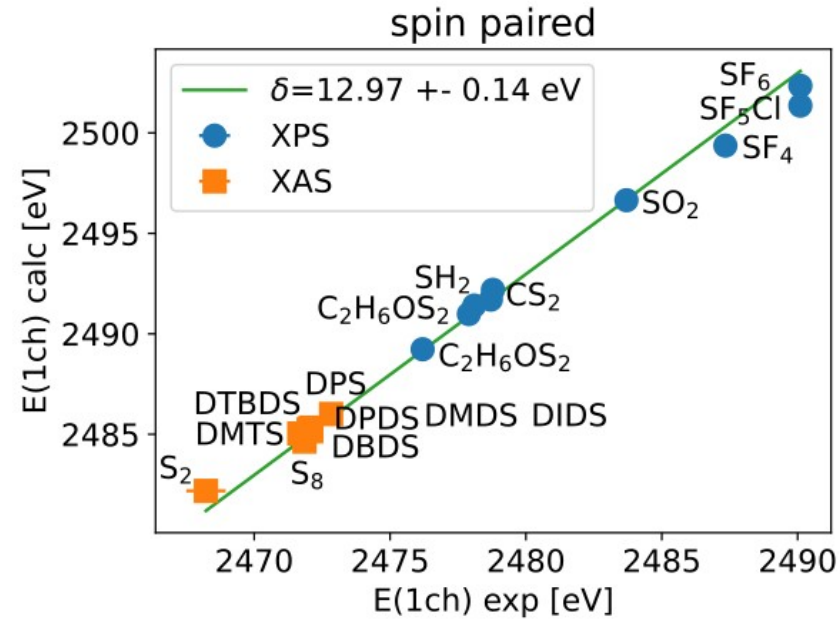
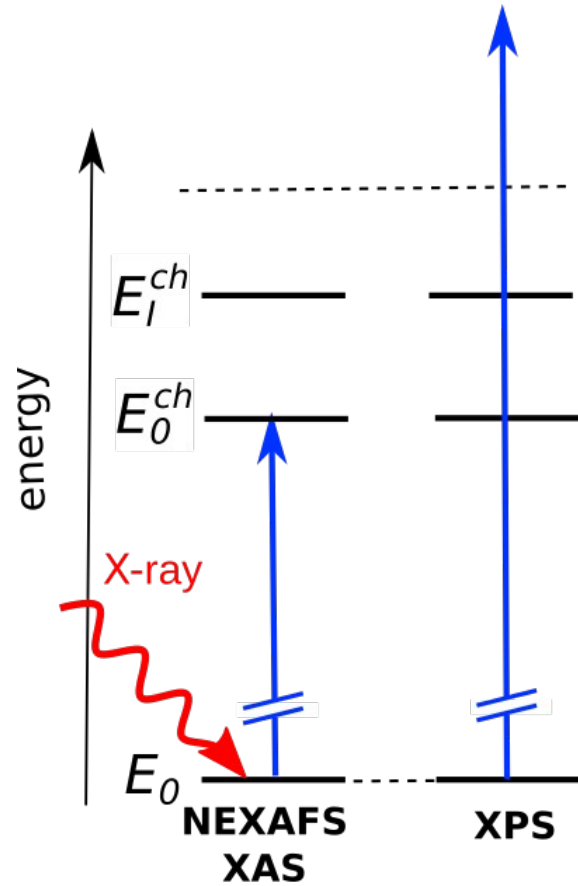


relative energies
less variation



X-ray absorption

S(1s) for gas-phase molecules



deKock et al PCCP 25 (2023) 20395

=> XPS and XAS require the same empirical shift

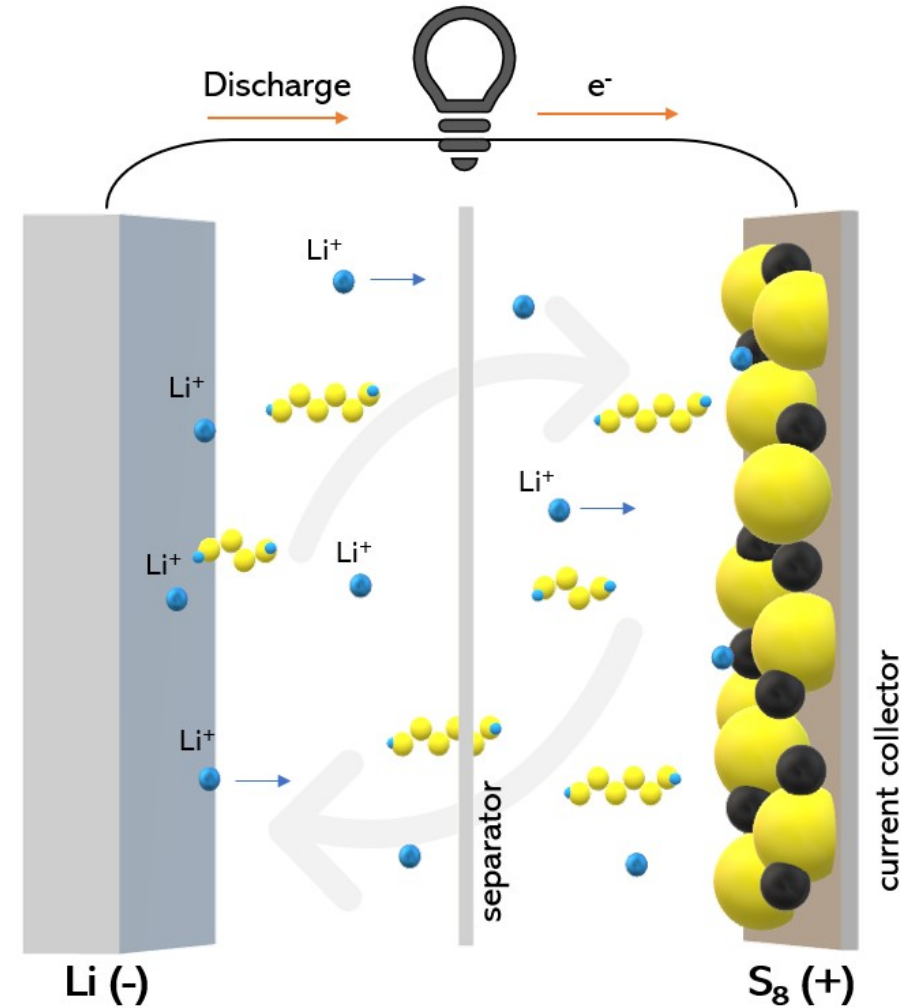


Application: LiS batteries



Chung et al. *Nat. Chem.* 5 (2018) 518

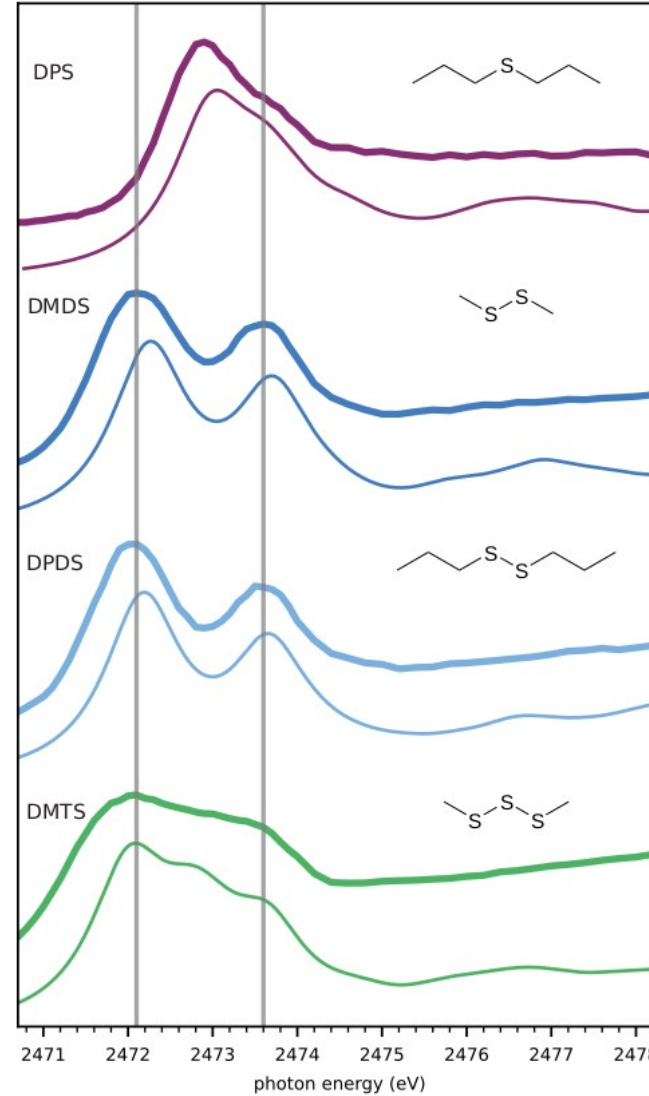
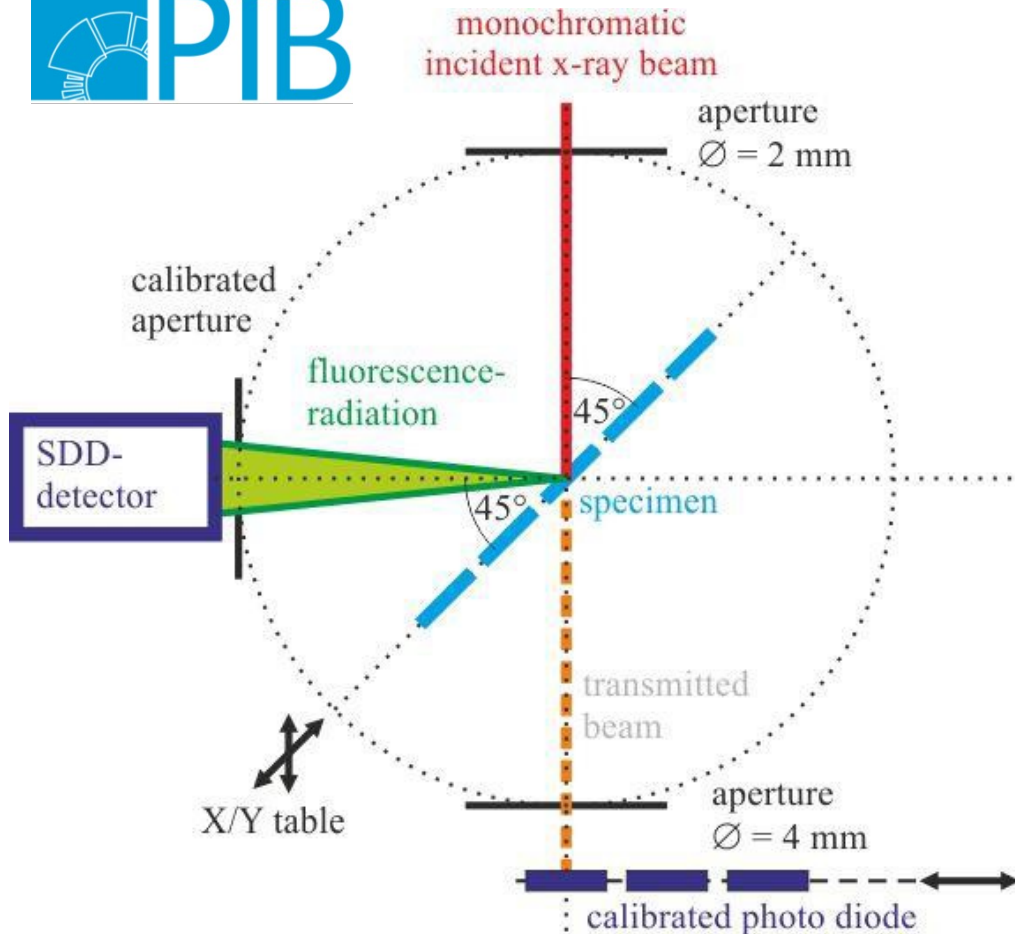
- highly abundant
- cheap
- replace Co



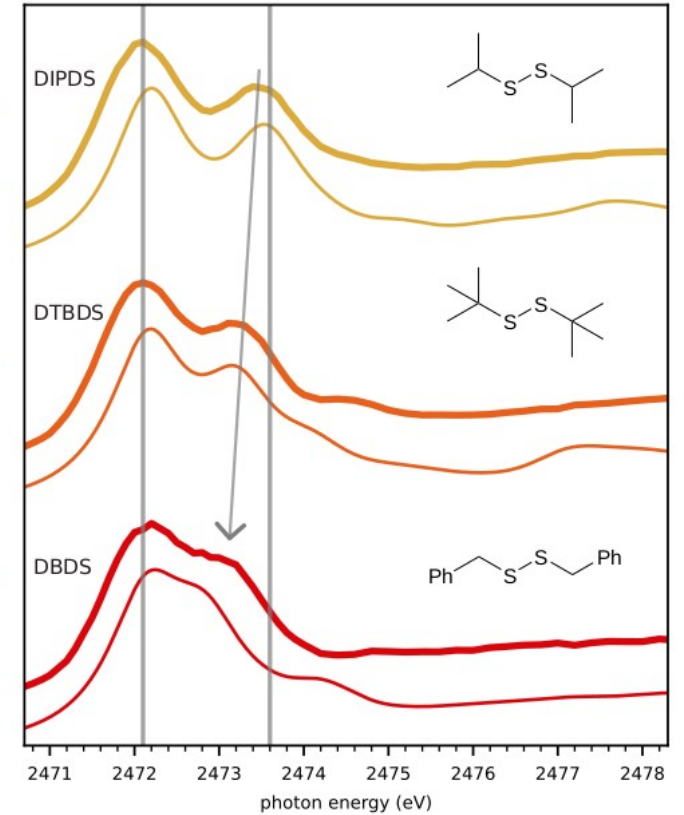
Source: wikipedia.org



Near edge x-ray fine structure experiments at PTB

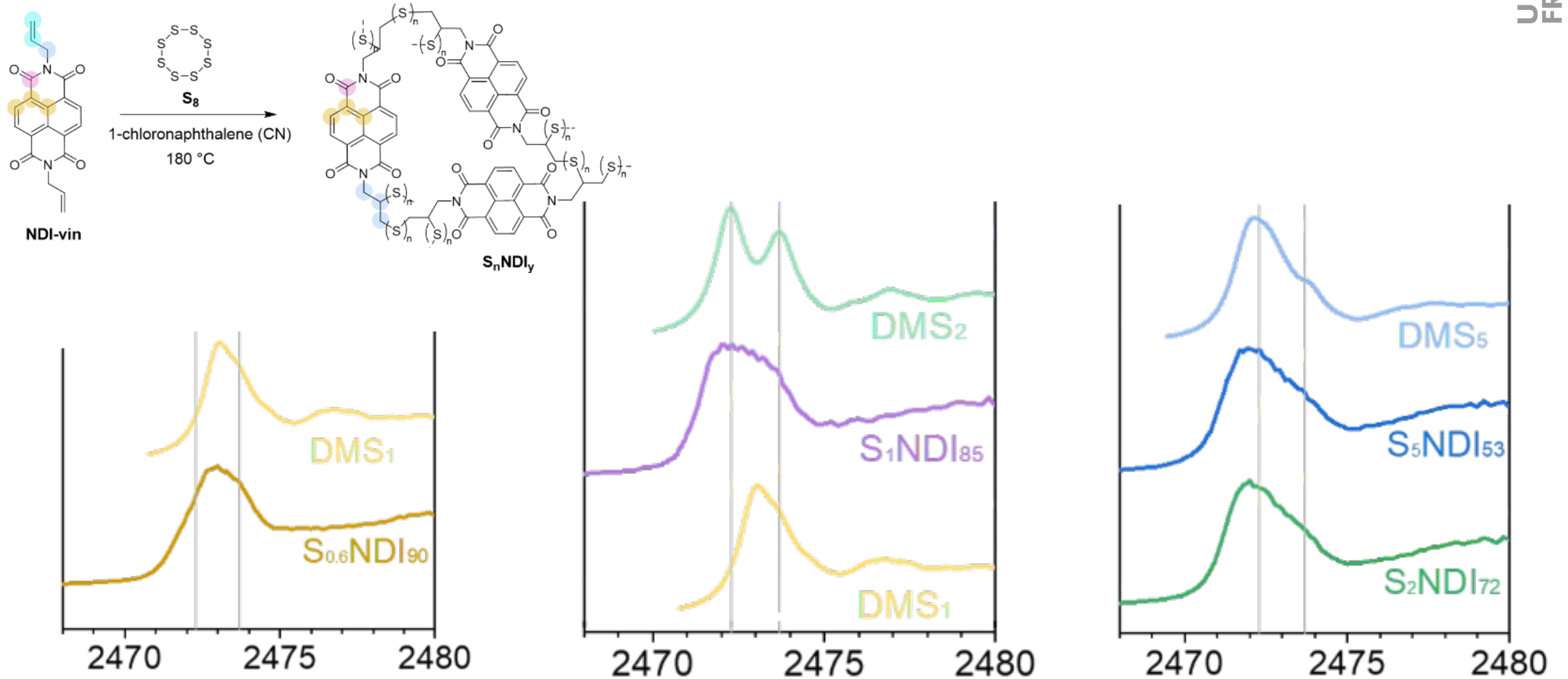


experiment
calculation





Application: S-strand lengths in Li-battery material





- GGA gives **excellent agreement** for gas phase XPS spectra
- Correction through **semi-empirical shift** to reveal **absolute energy scale** (solids require special care)
- XPS spectra reveal **structural information** of clusters
- The **same shift** appears in XAS spectra as in XPS
- NEXAFS spectra determine the **sulfur strand length** in novel battery materials



Thanks to



Group (FIT)

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livMatS



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