Ab initio simulations and X-ray spectroscopy: updates and perspectives

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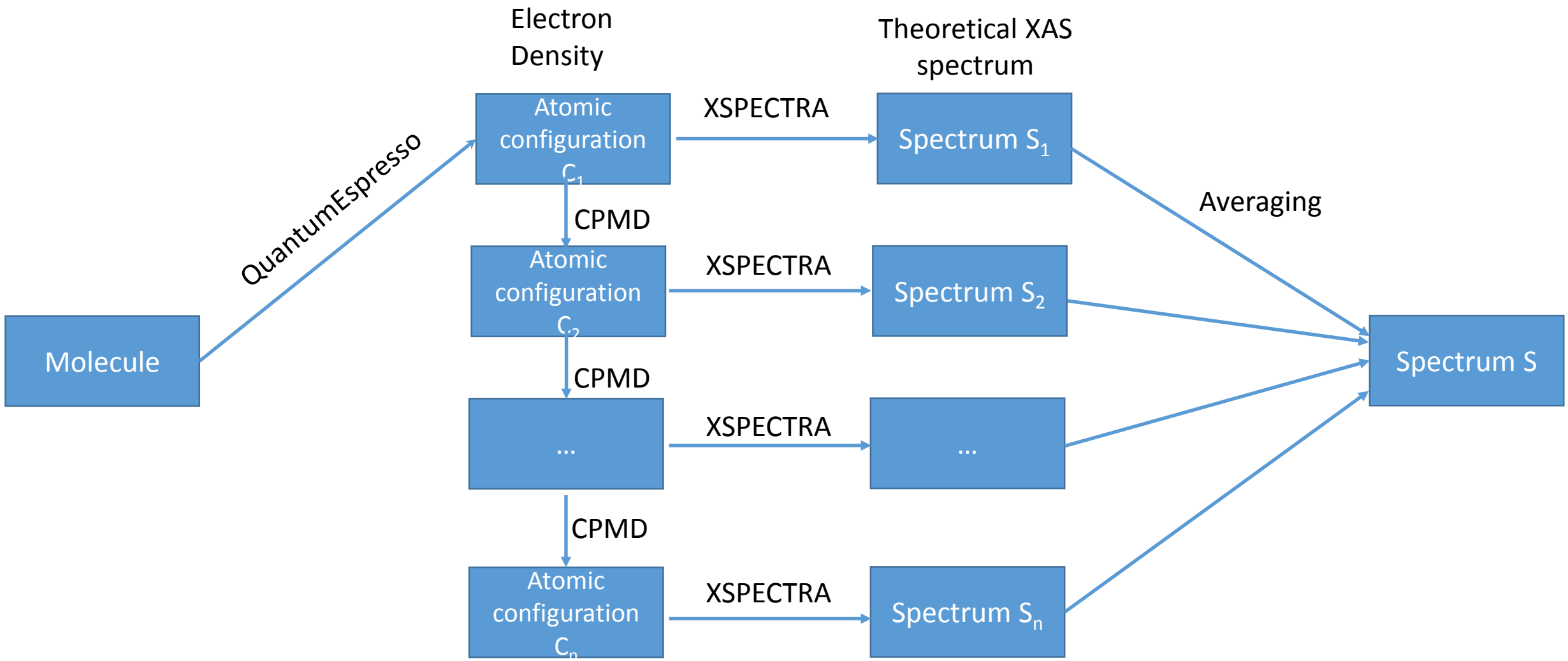
Ferrara, April 1st 2014

Outline

- X-ray Absorption Spectroscopy
  - A few paradigmatic cases
    - *Ab initio* calculations of XAS spectra
      - Semi-empirical calculations
        - Machines & Algorithms

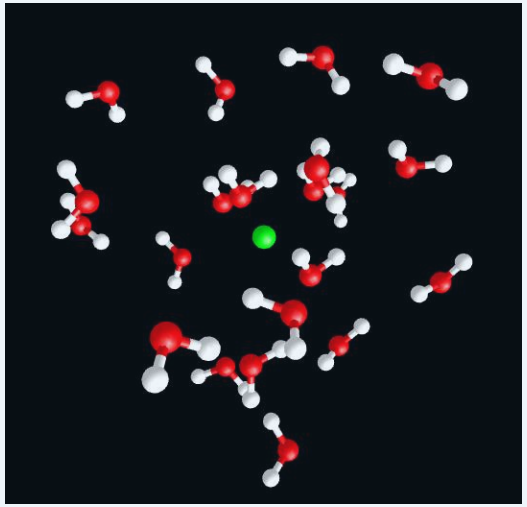
Ab initio XAS calculation flow-chart

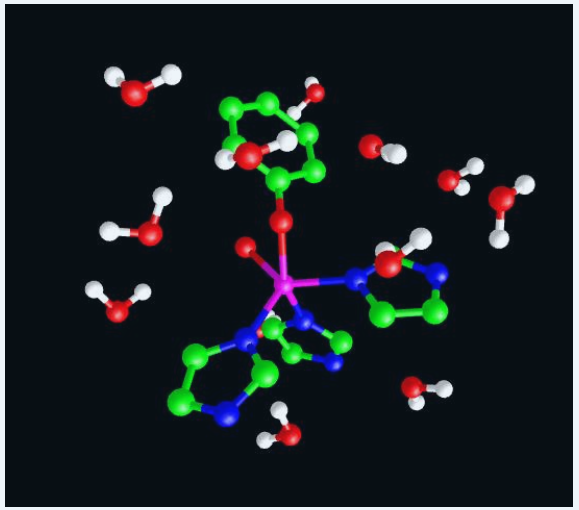


A few paradigmatic cases

Metallic copper

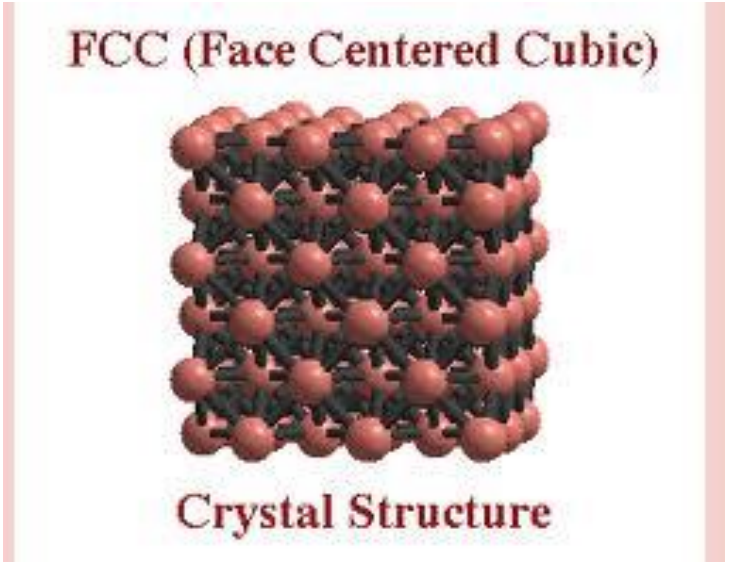
Cu(II) in water





Cu(II) in complex with peptides

A test-case: metallic Copper

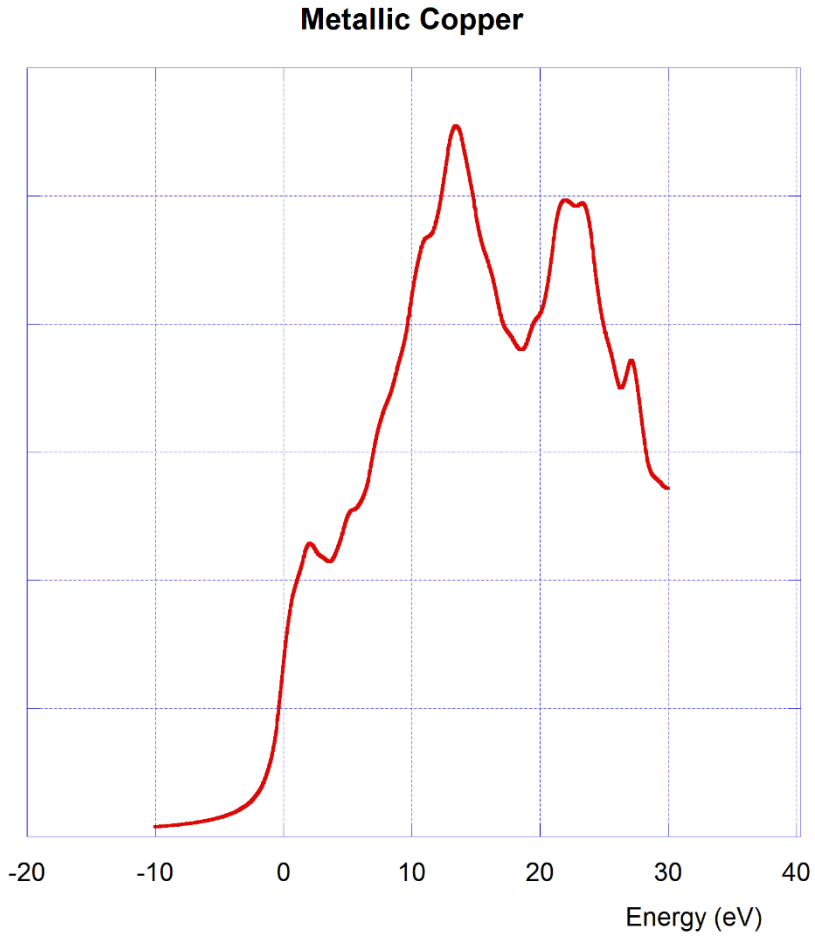


QuantumEspressso
Self-Consistent Field (SCF) relaxation

XSPECTRA cross-section calculation

FCC copper

XSPECTRA Calculation



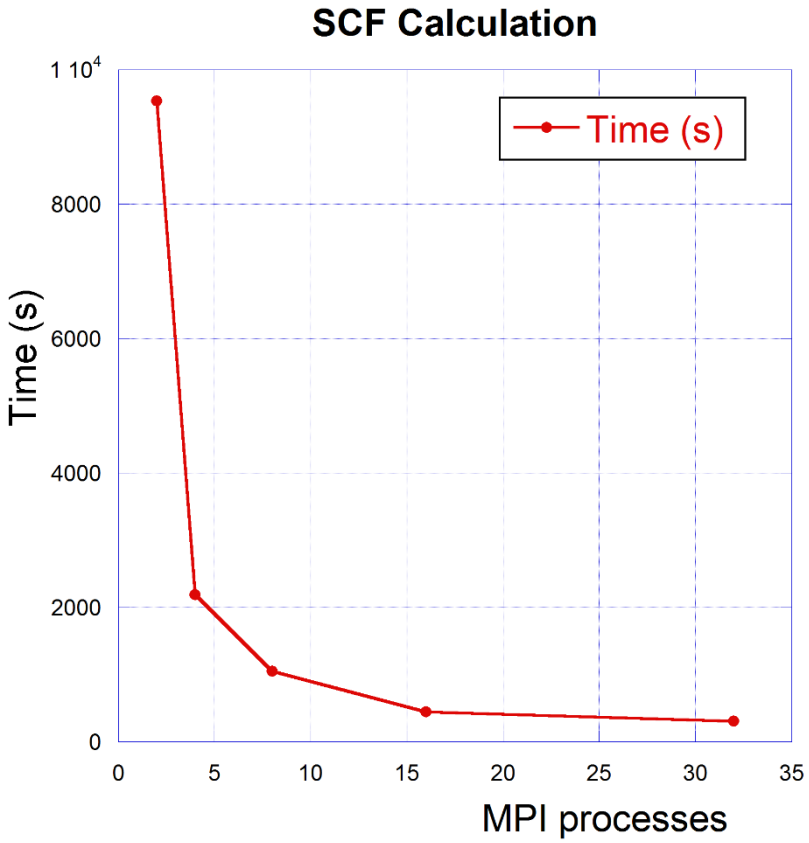
Gougoussis, Christos, et al. "First-principles calculations of x-ray absorption in a scheme based on ultrasoft pseudopotentials: from α-quartz to high-Tc compounds." *Physical Review B* 80.7 (2009): 075102.

A test-case: metallic Copper

QuantumESPRESSO
SCF calculation
Eurora @ cineca

MPI processes	CPU Time
32	5 m 4.73 s
16	7 m 25.63 s
8	17 m 29.16 s
4	36 m 26.91 s
2	2 h 39 m

10 Å cell
27 atoms

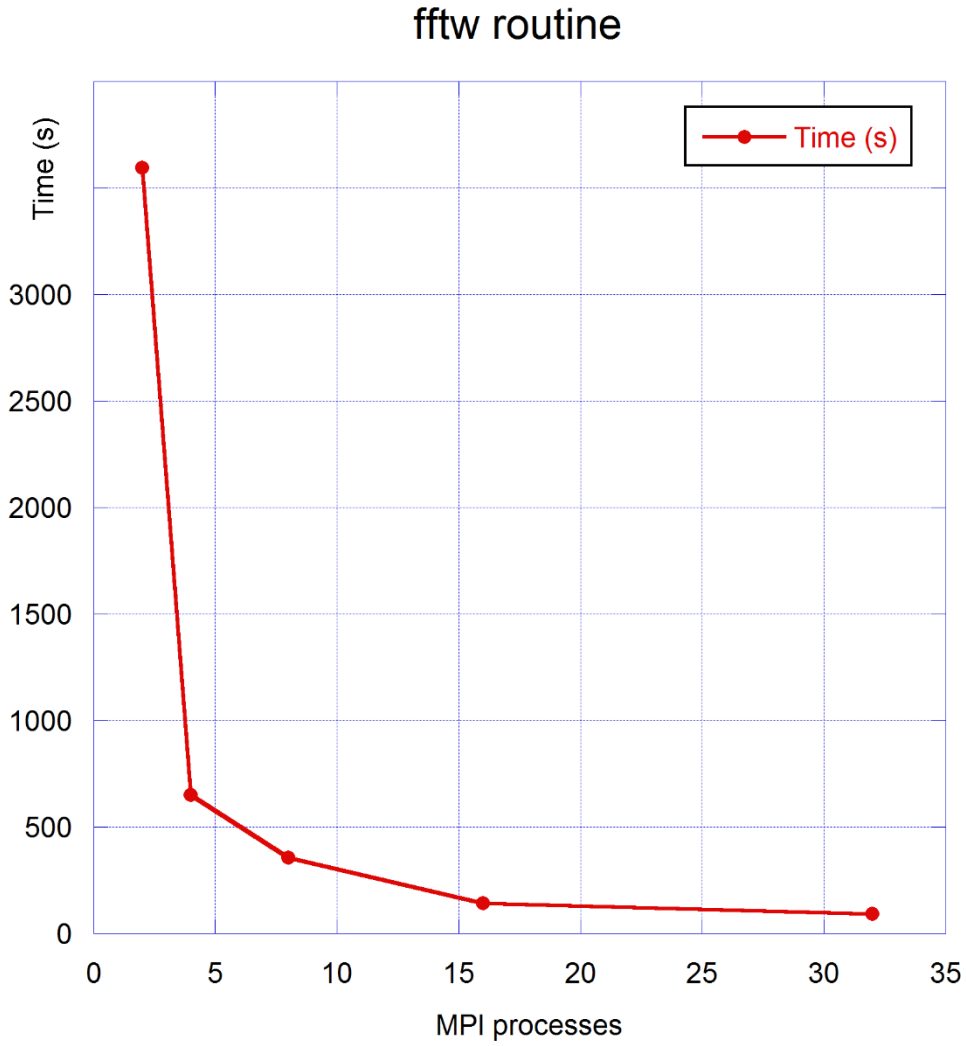


A test-case: metallic Copper

QuantumESPRESSO
fft calculation
Eurora @ cineca

MPI processes	CPU Time
32	91.00 s
16	142.93 s
8	356.39 s
4	651.07 s
2	3595.00 s

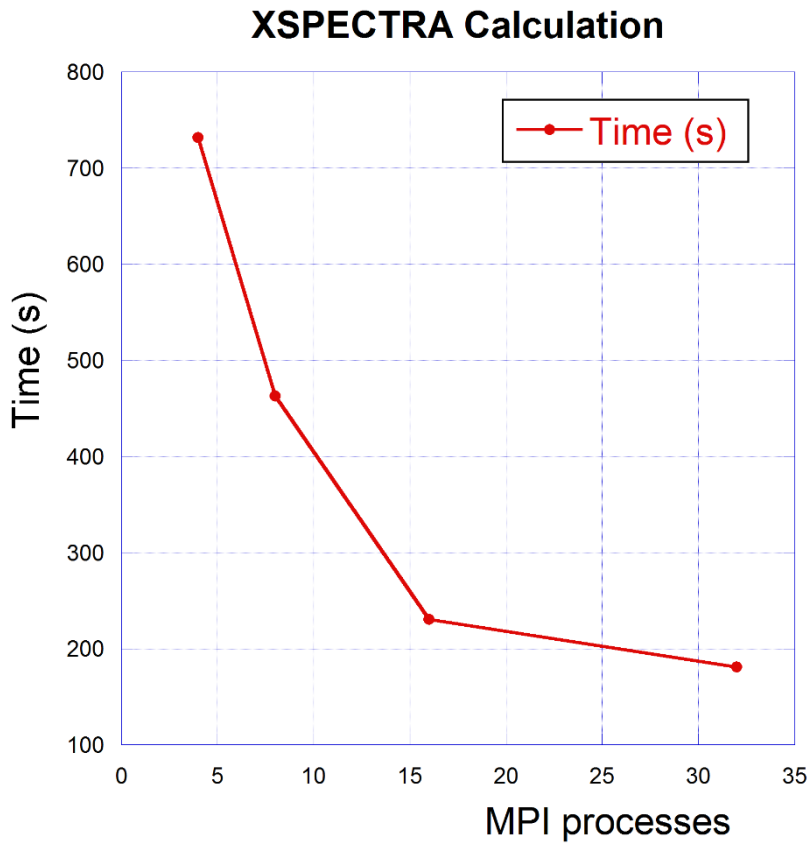
10 Å cell
27 atoms



A test-case: metallic Copper

XSPECTRA
XANES calculation
Eurora @ cineca

MPI processes	CPU Time
32	180.95 s
16	230.13 s
8	462.65 s
4	731.27 s



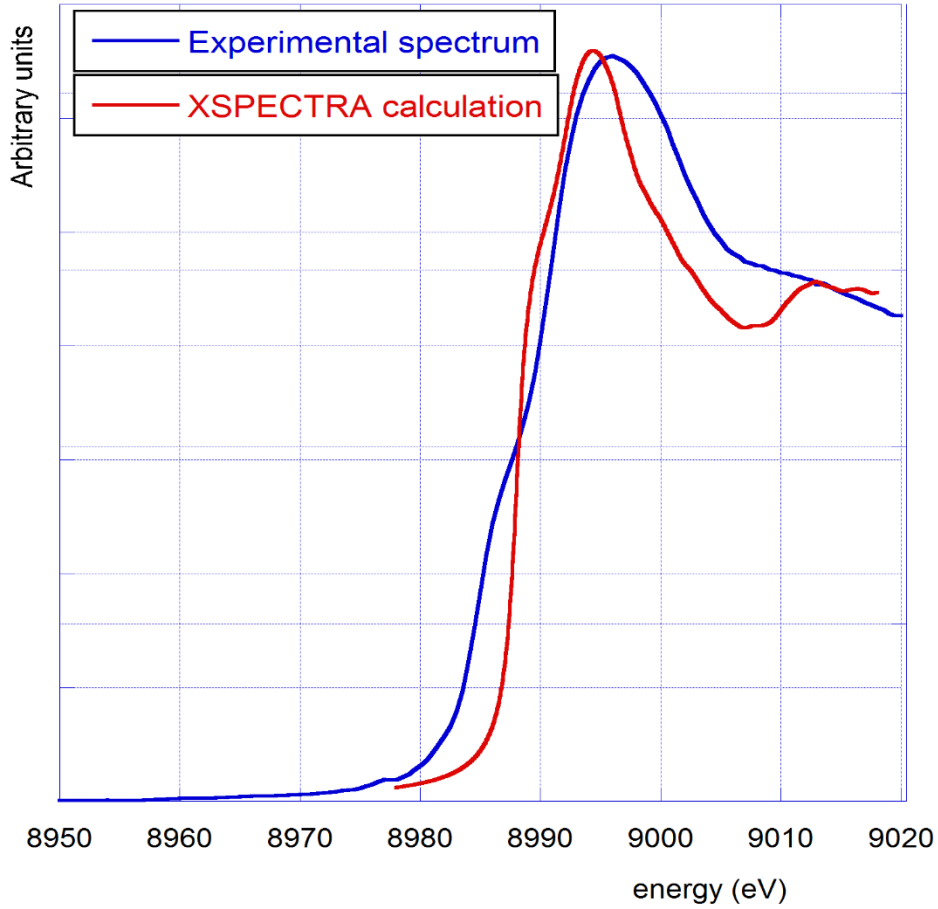
Experimental data: Copper in water

QuantumEspressso
SCF relaxation

XSPECTRA Calculation
of cross-section

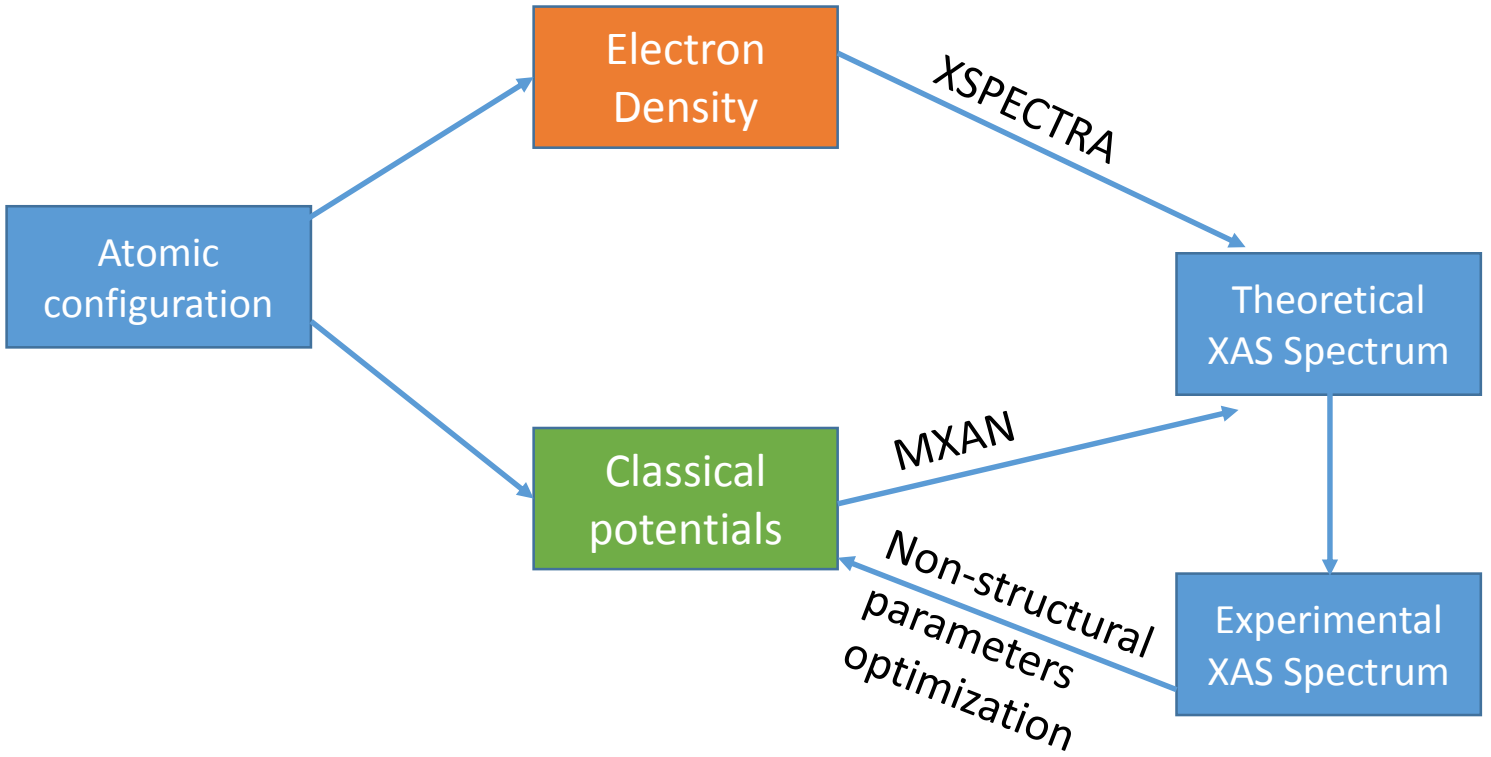
Cu(II) in water

20 Å cell
88 atoms



Good agreement with
experimental data

Ab initio vs semi-empirical XAS calculations



Ab initio calculation
Computationally expensive

Semi-empirical calculation
Computationally faster (1 min on a PC)
Easy to compare with experiments

Machines & algorithms

Machine	Gromacs	DFTB+	QuantumEspresso	XSPECTRA	MXAN
PC	√	√	√	√	√
Eurora	√	o	√	√	o
Fermi	√	√	√	√	o
Zefiro	√	o	√	(√)	o

Thank you
for your attention