

X-ray (XPS and XAS) analysis of pyrite thin films

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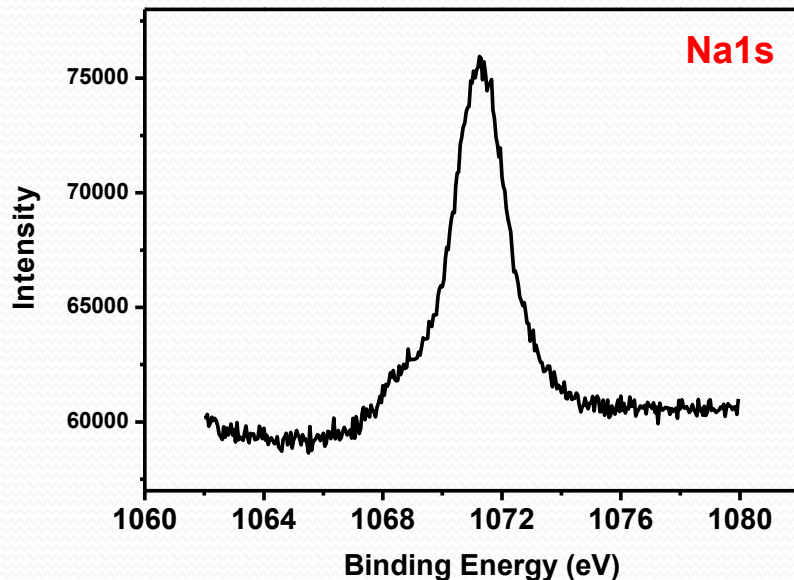
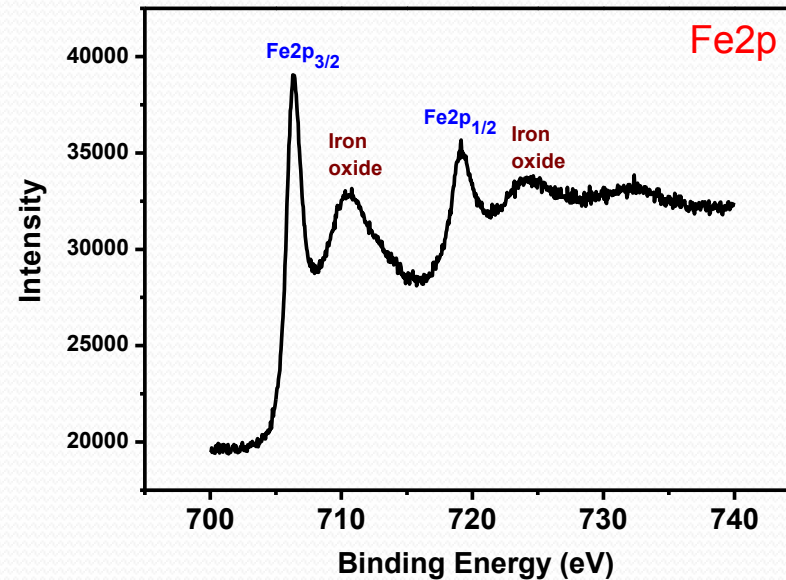
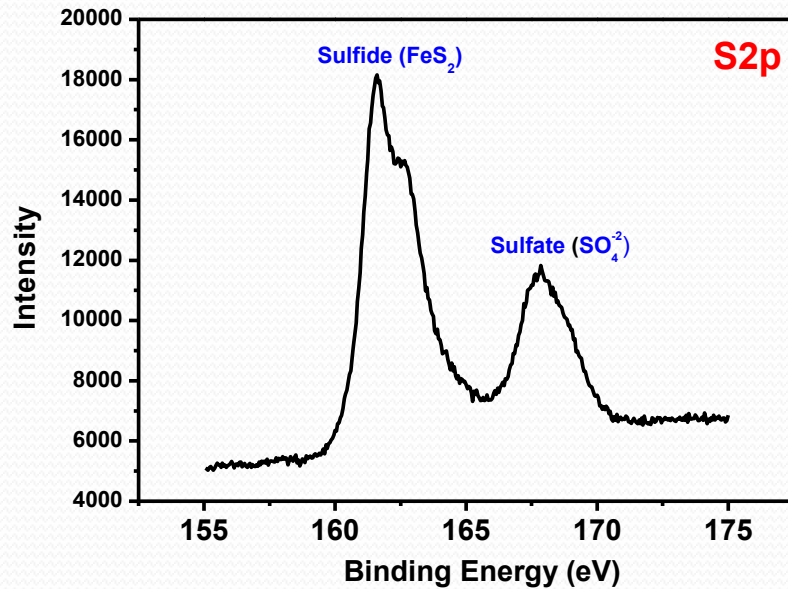
John C. Hemminger group

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Outline

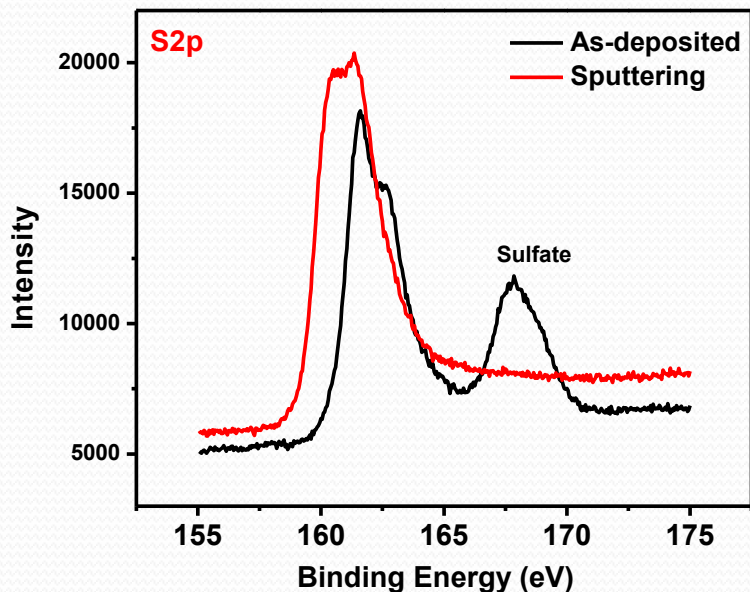
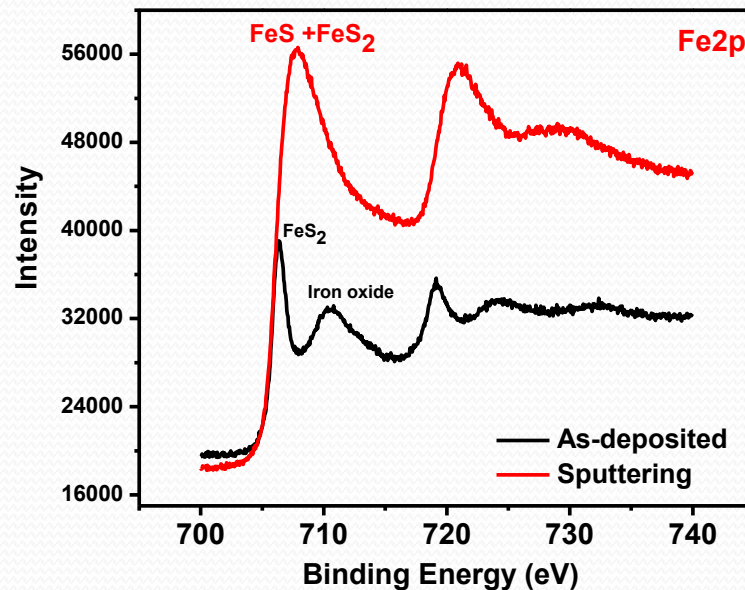
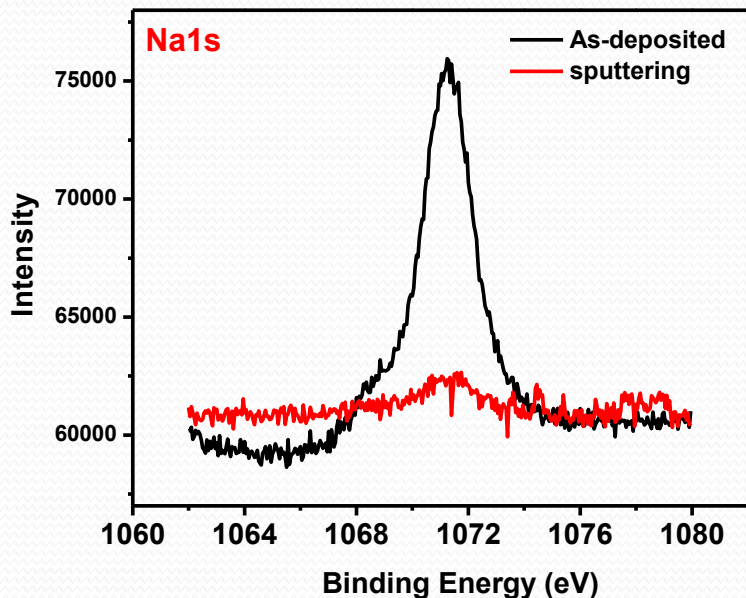
- **Pyrite thin films on the glass**
 - Remove Na from the surface
- **Pyrite thin films on Si**
 - Remove elemental sulfur on the surface
 - Band gap determination from X-ray absorption (XAS) and XPS.

Pyrite thin films on the glass



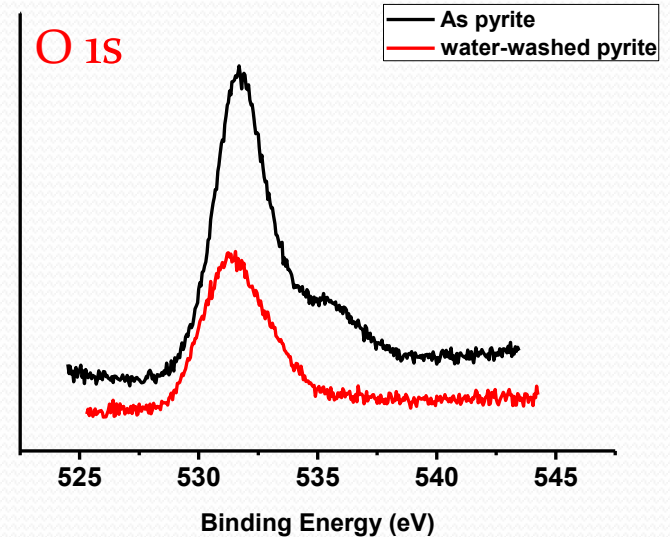
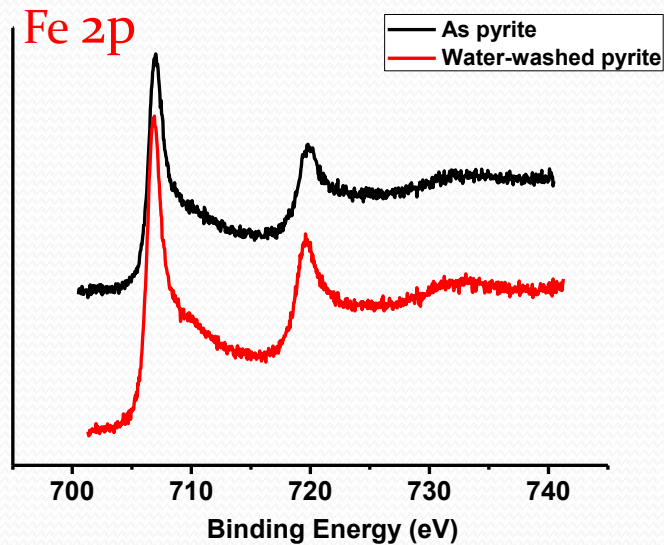
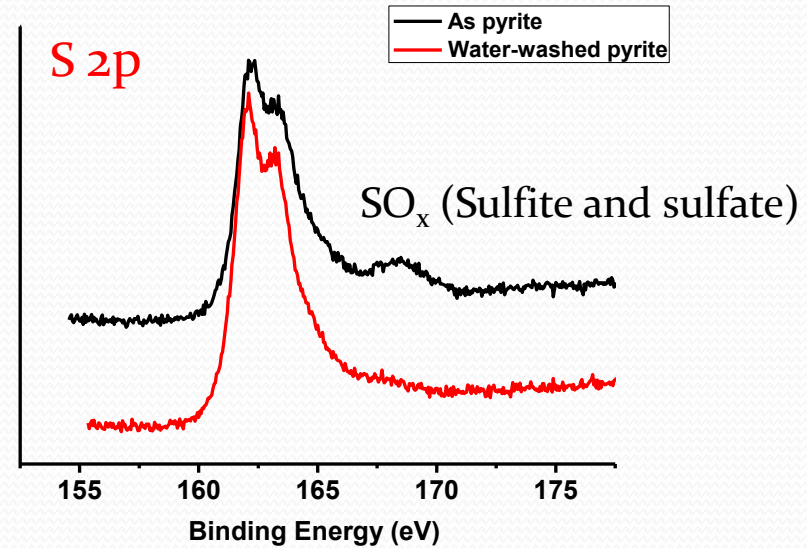
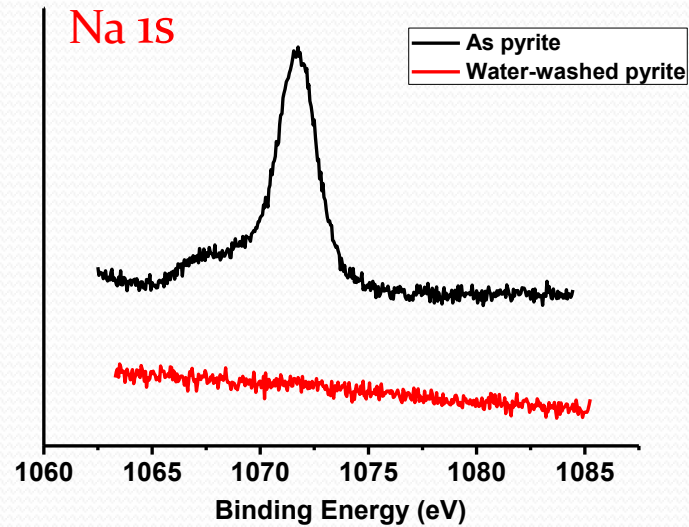
- The pyrite has been **oxidized**.
- **Na exists** on the surface of the pyrite thin film.

Ar Sputtering changes the surface composition

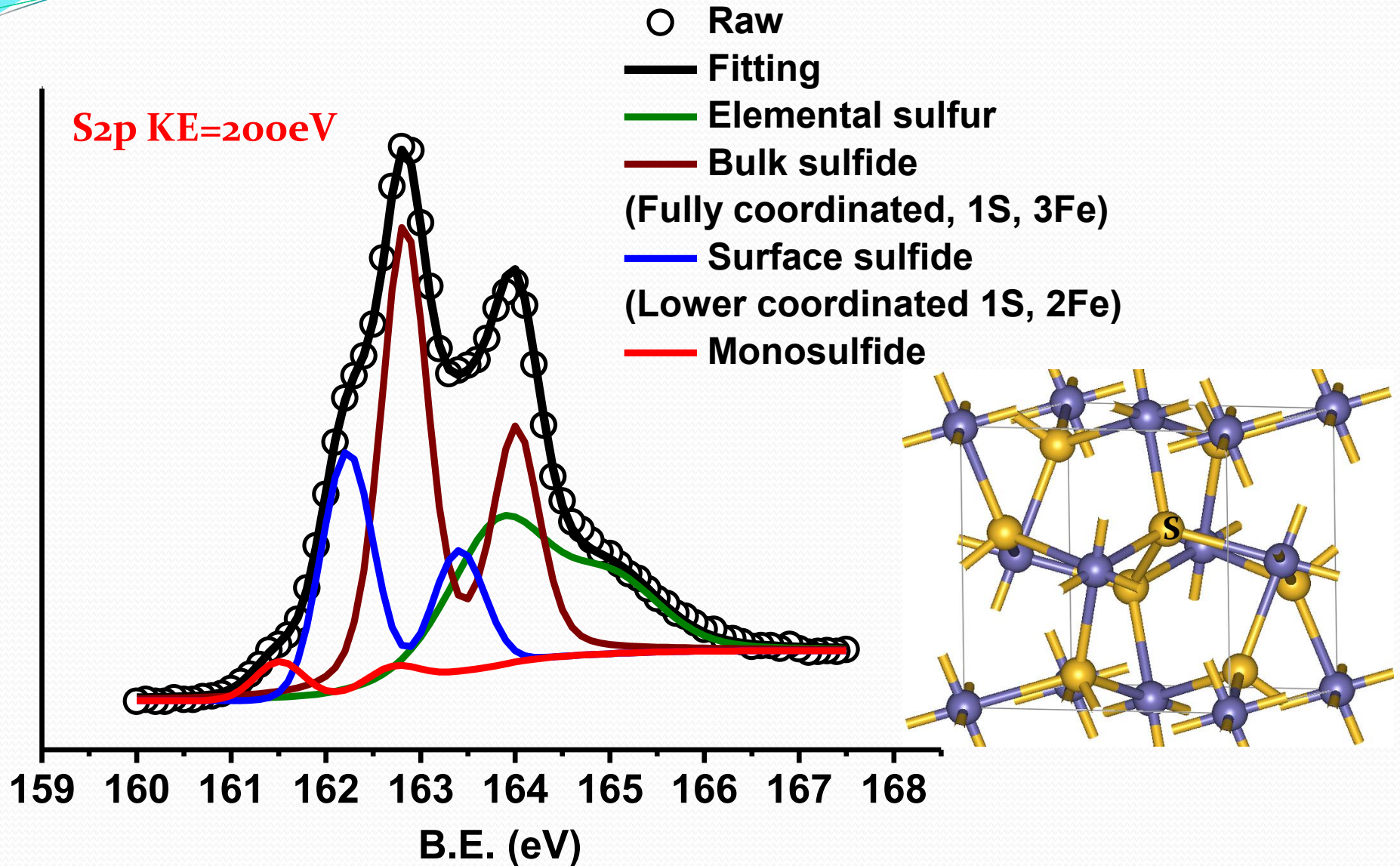


- **Sputtering condition:** 5×10^{-5} torr Ar, 2 KV (beam energy), 20mA (emission current), 5 mins.
- **Na is removed** by Ar sputtering which indicates Na only exists on the surface.
- **The broadening** of Fe 2p and S2p peaks after Ar sputtering is attributed to **sulfur preferential sputtering**.

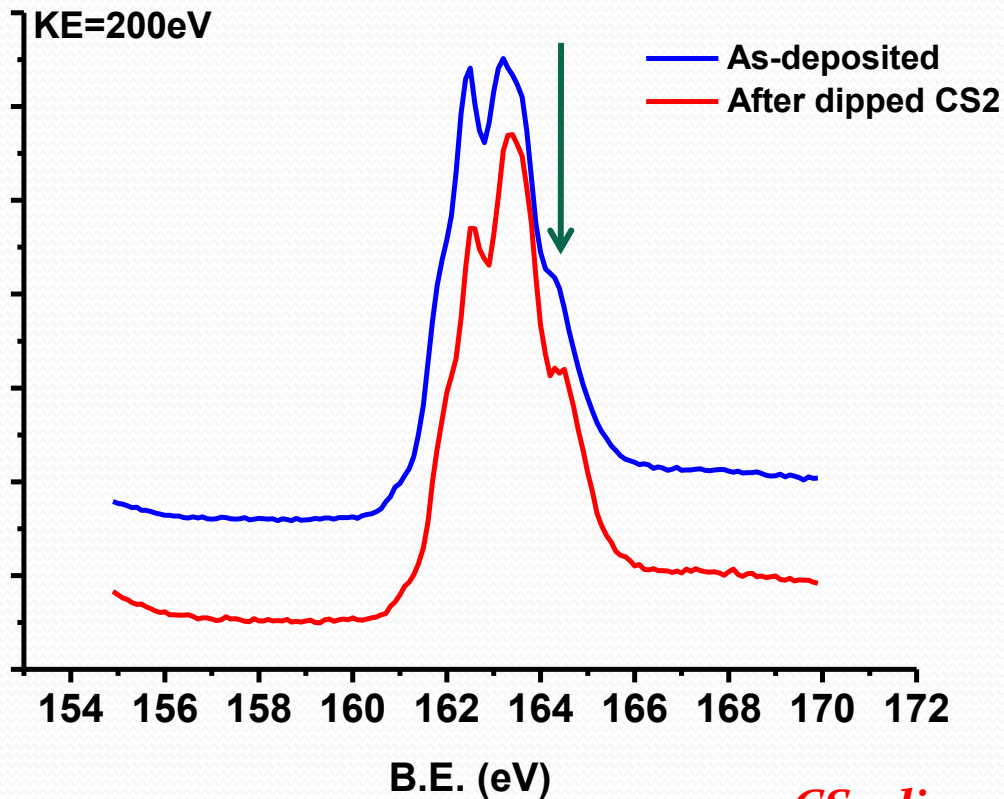
Water remove Na from the surface of pyrite on the glass



Surface structure of Pyrite thin films on Si



As-deposited V.S. CS₂ dipped pyrite on Si

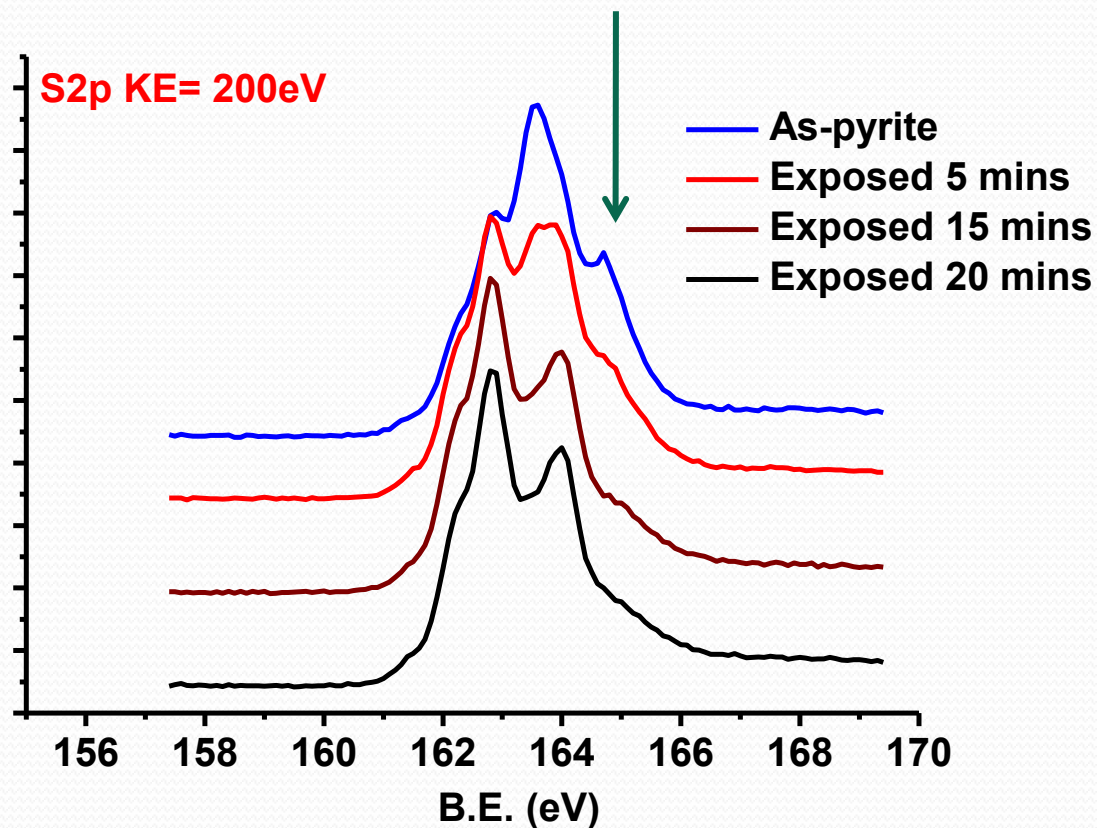


Extraction and Quantitative Analysis
of Elemental Sulfur from Sulfide
Mineral Surfaces by
High-Performance Liquid
Chromatography

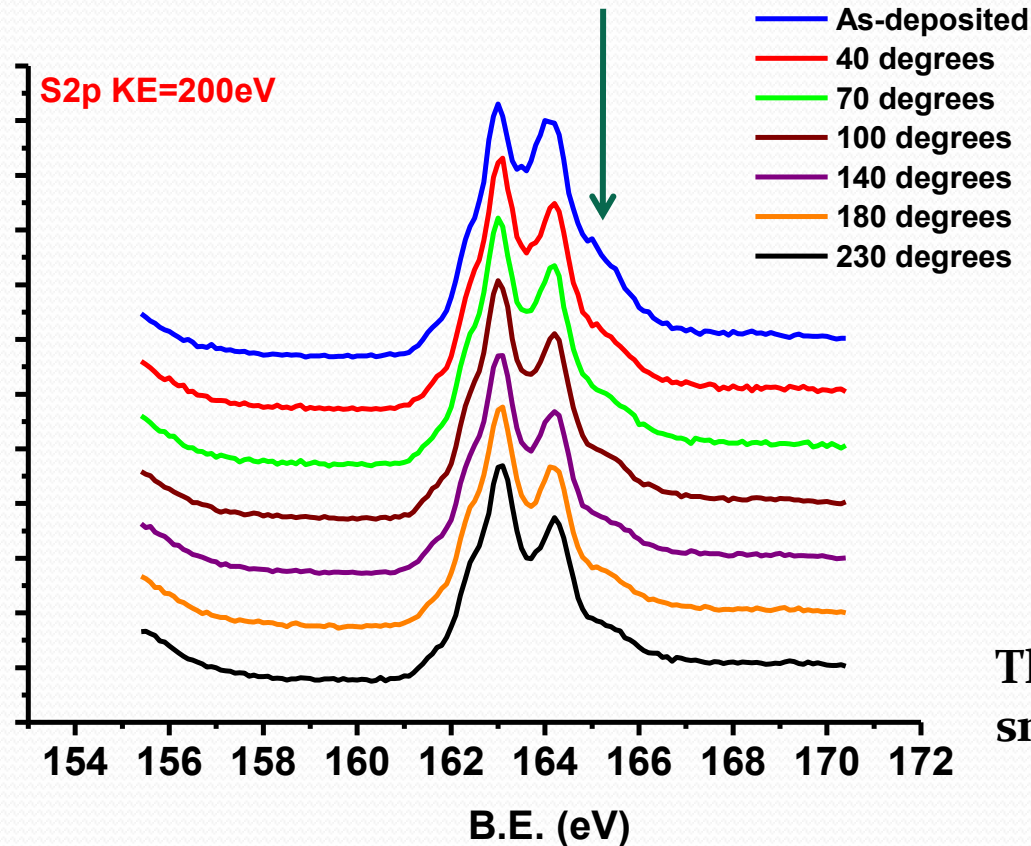
Environ. Sci. Technol. 2000, 34, 4651–4655

CS₂ dipped method did not work.

X-ray radiation remove elemental sulfur for pyrite on the Si

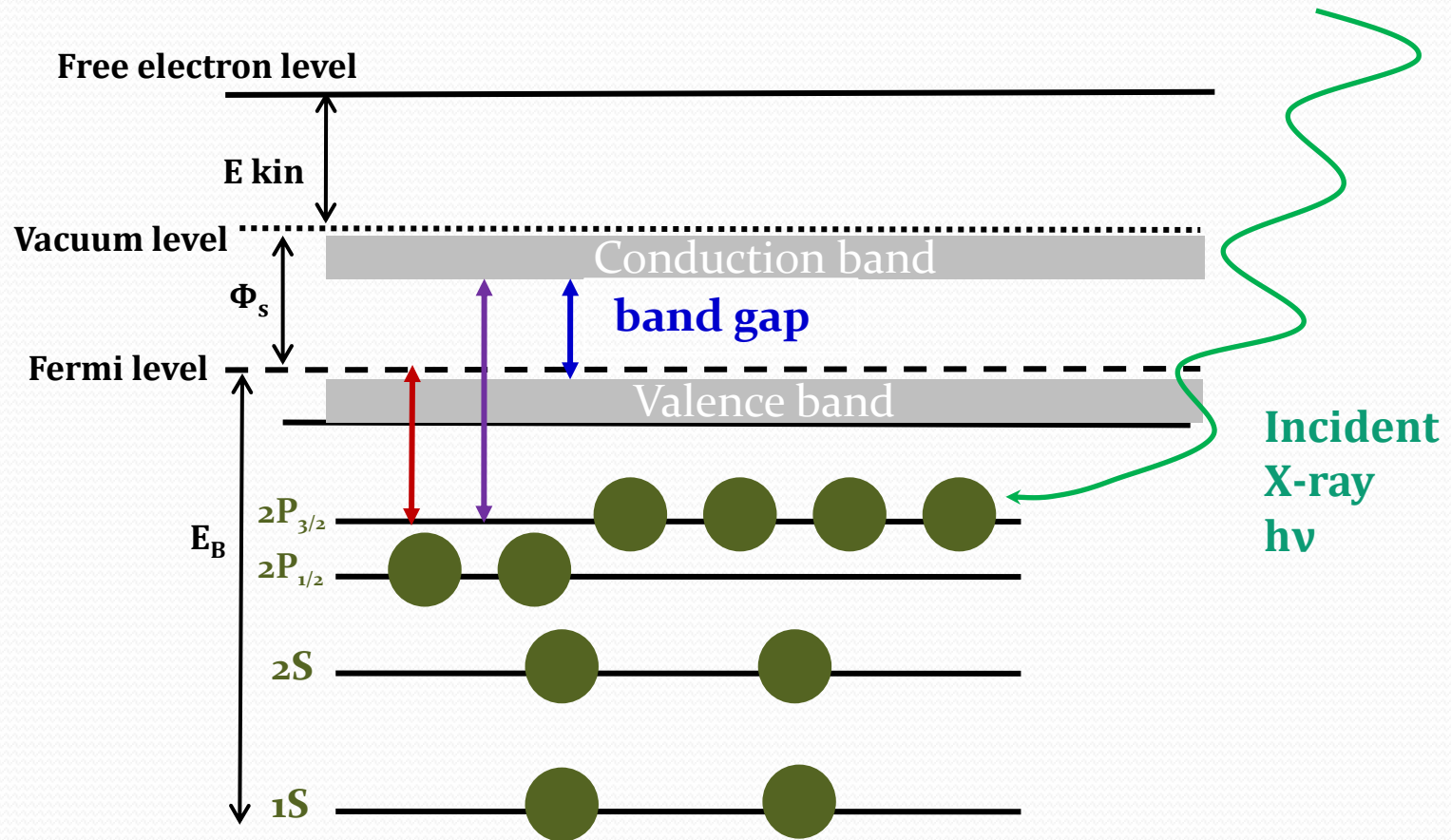


Heating further remove elemental sulfur for pyrite on Si



The surface still contains small amount of sulfur species.

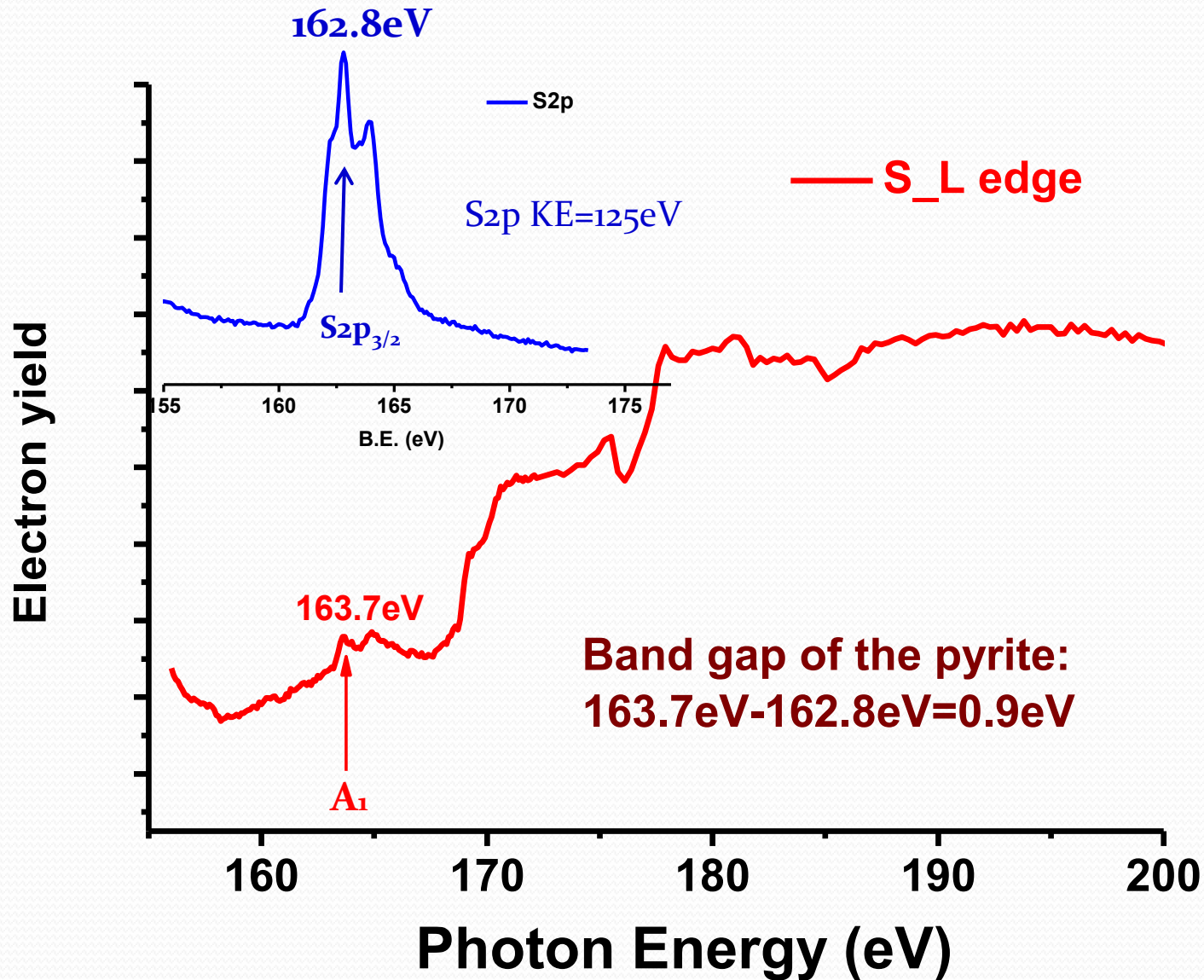
XPS and XAS energy level diagram



XPS: $E_{kin} = h\nu - E_B - \Phi_s$ For example, E_B for $S2p_{3/2}$

XAS: Electrons from core level to unoccupied conduction band, For example, A_1 for S_L edge

Band gap determination



Take-home messages

- **Pyrite thin films on the glass**
 - **water** is able to move Na and SO_x from the surface
- **Pyrite thin films on Si**
 - **X-ray radiation** and **heating** can remove elemental sulfur on the surface.
 - Band gap is about **0.9eV** determined from X-ray absorption (XAS) and XPS.

Future work:

- Determination of pyrite stoichiometry (Fe_yS_x)
- More precisely determinate band gap by calibrating beamline photon energies.