

This readme file was generated on 2025-01-08 by Elin Cartwright

GENERAL INFORMATION

Title of Dataset: Resonant Auger Spectroscopy and Hard X-ray Photoelectron Spectroscopy data of lead-containing materials (PbS quantum dots of sized 2, 3 and 5nm, PbS bulk reference, PbS Galena crystal, PbI₂ reference)

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Date of data collection: 2021-05-11 – 2024-08-30

Geographic location of data collection: HZB BESSY II synchrotron (Berlin, Germany)

Information about funding sources that supported the collection of the data: This research has been funded by the Swedish Research Council and the Wallenberg Initiative Materials Science for Sustainability (WISE) funded by the Knut and Alice Wallenberg Foundation.

DATA & FILE OVERVIEW

File List:

Resonant Auger 2D maps file list:

(The first wave in each file is the photon energy axis, the following rows are Auger spectra in the Pb MNN region over the photon energies in the first row).

RAS_PbSQD2nm.txt

RAS_PbSQD3nm.txt

RAS_PbSQD5nm.txt

RAS_PbSbulk.txt

RAS_PbSGalena.txt

RAS_PbI2.txt

HAXPES measurements file list:

(The first column is the calibrated binding energy [eV] and the second column is the intensity [arb. Units])

HAXPES_I4d_PbSQD2nm.txt (Measurement of valence region and I4d core-level)

HAXPES_I4d_PbSQD3nm.txt (Measurement of valence region and I4d core-level)

HAXPES_I4d_PbSQD5nm.txt (Measurement of valence region and I4d core-level)

HAXPES_I4d_PbI2.txt (Measurement of valence region and I4d core-level)

HAXPES_Pb4f_S2p_PbSQD2nm.txt (Measurement of Pb4f and S2p core-levels)

HAXPES_Pb4f_S2p_PbSQD3nm.txt (Measurement of Pb4f and S2p core-levels)

HAXPES_Pb4f_S2p_PbSQD5nm.txt (Measurement of Pb4f and S2p core-levels)

HAXPES_Pb4f_S2p_PbSbulk.txt (Measurement of Pb4f and S2p core-levels)

HAXPES_Pb4f_S2p_PbSGalena.txt (Measurement of Pb4f and S2p core-levels)

HAXPES_Pb4f_S2p_PbI2.txt (Measurement of Pb4f and S2p core-levels)

METHODOLOGICAL INFORMATION

Description of methods used for collection/generation of data: Resonant Auger maps were collected by measuring Auger spectra in the Pb MNN electron kinetic energy region for multiple photon energies over the Pb M-edge. The measurements were conducted at the High Kinetic Energy (HIKE) end-station at the KMC-1 beamline at the synchrotron BESSY II, using a Scienta R4000 hemispherical electron energy analyzer.

Methods for processing the data: Collected data files have been loaded into Igor Pro 7.08 and calibrated using the method described below.

Software-specific information needed to interpret the data: Load files into Igor Pro (any version) as General text files. To fit spectroscopic data, the CurveFitting procedure (SPANCF) by Edwin Kukk can be used.

Calibration information: All spectra are calibrated by the Au 4f binding energy of 84.0 eV, using a measurement of a gold foil at the same photon as each spectrum.

DATA-SPECIFIC INFORMATION FOR FILES WITH NAME: RAS_...

Variable List: photon energy (eV), electron kinetic energy (eV), intensity (arb. units)

DATA-SPECIFIC INFORMATION FOR FILES WITH NAME: HAXPES_...

Variable List: binding energy (eV) and intensity (arb. units)