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Cadmium selenide by XPS

Rogelio Ospina^{1,a)}, Sergio A. Rincón-Ortiz¹ and Jhonatan Rodriguez-Pereira^{1,2}

¹Centro de Investigación Científica y Tecnológica en Materiales y Nanociencias (CMN), Universidad Industrial de Santander, Piedecuesta, Santander, P.C. 681011, Colombia.

²Center of Materials and Nanotechnologies, Faculty of Chemical Technology, University of Pardubice, Nam. Cs. Legii 565, 53002 Pardubice, Czech Republic.

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Cadmium selenide was analyzed using x-ray photoelectron spectroscopy (XPS). The specimen is a powder purchased from Chemsavers. Sample was fixed to a stainless-steel sample holder with copper 3M™ double-sided adhesive tape. Survey spectra, Cd 3d, Se 3d, O 1s, Cd 3p, Cd MNN, Se LMM, Se 3p, C 1s, and Cd 4d core level along with the valence band spectra were recorded. Results point out a stoichiometry of 0.95 on surface.

Keywords: CdSe; XPS; metal chalcogenide, semiconductor

INTRODUCTION

Due to their optical and electrical properties, metal chalcogenides are materials that can be used in different optoelectronic applications, as well as in electronic devices (transistors, diodes, etc.). Metal chalcogenides are chemical compounds between a transition metal and an anion chalcogen (S, Se, Te) (Refs 1-4). In this work, a sample of cadmium selenide (CdSe) was analyzed, which is a very popular material in this area because it has a band gap energy of 1.74 eV (Ref. 4).

SPECIMEN DESCRIPTION (ACCESSION # 01637)

Host Material: CdSe

CAS Registry #: 1306-24-7

Host Material Characteristics: homogeneous; solid; polycrystalline; semiconductor; semiconductor; Powder

Chemical Name: Cadmium selenide

Source: Chemsavers

Host Composition: CdSe (99.999%)

Form: Powder

Structure: CdSe

History & Significance: CdSe powder was ground and fixed to a sample holder with copper 3M™ double-sided adhesive tape.

As Received Condition: As powder

Analyzed Region: same as host material

Ex Situ Preparation/Mounting: As received.

In Situ Preparation: None

Charge Control: Not applicable

Temp. During Analysis: 300 K

Pressure During Analysis: $< 1 \times 10^{-7}$ Pa

Pre-analysis Beam Exposure: Not applicable s

Accession#: 01637

Technique: XPS

Host Material: CdSe

Instrument: SPECS PHOIBOS 150

Major Elements in Spectra: Cd, Se

Minor Elements in Spectra: C, O

Published Spectra: 9

Spectra in Electronic Record: 9

Spectral Category: comparison

INSTRUMENT DESCRIPTION

Manufacturer and Model: SPECS PHOIBOS 150 - SPECS Surface Nano Analysis GmbH

Analyzer Type: spherical sector

Detector: other

Number of Detector Elements: 25

INSTRUMENT PARAMETERS COMMON TO ALL SPECTRA

■ Spectrometer

Analyzer Mode: constant pass energy

Throughput (T=E^N): N=0

Excitation Source Window: Mylar window, allows high X-ray transmission: 88% for Al K α .

Excitation Source: Al K α monochromatic

Source Energy: 1486.6 eV

Source Strength: 200 W

Source Beam Size: 2000 μ m x 2000 μ m

Signal Mode: multichannel direct

■ Geometry

Incident Angle: 55 °

Source-to-Analyzer Angle: 55 °

Emission Angle: 0 °

Specimen Azimuthal Angle: Not applicable

Acceptance Angle from Analyzer Axis: 16 °

Analyzer Angular Acceptance Width: 16 ° x 16 °

■ Ion Gun

Manufacturer and Model: SPECS IQE 12/38

Energy: 5000 eV

^{a)}Electronic mail: rospinao@uis.edu.co

Current: 70 mA

Current Measurement Method: biased stage

Sputtering Species: Ar⁺

Spot Size (unrastered): 3000 μm x 3000 μm

Raster Size: Not applicable μm x μm

Incident Angle: 54 °

Polar Angle: Not applicable

Azimuthal Angle: Not applicable

Comment: The specimen was analyzed as loaded. The ion gun was used only for cleaning the Ag reference foil.

DATA ANALYSIS METHOD

Energy Scale Correction: Binding energy scale was referenced to Cd 3d_{5/2} = 405.0 (Ref. 5).

Recommended Energy Scale Shift: -0.11 eV

Peak Shape and Background Method: Peak position and width were determined from fitting the spectra using a mixed Gaussian– Lorentzian function after subtraction of a Shirley background using the CasaXPS Software.

Quantitation Method: Peak areas were obtained from fitting the spectra and relative sensitivity factors from the atomic photoionization cross section of each core level provided by SPECS Prodigy library.

ACKNOWLEDGMENTS

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SPECTRAL FEATURES TABLE							
Spectrum ID #	Element/ Transition	Peak Energy (eV)	Peak Width FWHM (eV)	Peak Area (eV x cts/s)	Sensitivity Factor	Concentration (at. %)	Peak Assignment
01637-02	Cd 3d	1.94x10 ⁴	19.84	41.77	...
01637-02	Cd 3d _{5/2}	405.0	0.88	CdSe
01637-02	Cd 3d _{3/2}	411.7	0.86	CdSe
01637-03	Se 3d	2.42x10 ³	2.41	39.63	...
01637-03	Se 3d _{5/2}	53.8	0.92	CdSe
01637-03	Se 3d _{3/2}	54.6	0.87	CdSe
01637-04	O 1s	531.5	2.50	9.45x10 ²	2.77	18.60	Contaminant
01637-05	Cd 3p _{3/2}	617.9	3.49	8.92x10 ³	CdSe
01637-05	Cd 3p _{1/2}	651.8	3.40	4.46x10 ³	CdSe
01637-06 ^a	Cd MNN	375.3	3.74	3.53x10 ³	CdSe
01637-06 ^a	Cd MNN	381.9	1.88	1.50 x10 ³	CdSe
01637-07 ^a	Se LMM	1307.2	2.32	1.43x10 ⁴	CdSe
01637-07	Se 3p _{3/2}	160.2	1.89	2.26x10 ³	CdSe
01637-07	Se 3p _{1/2}	165.9	1.70	1.04x10 ³	CdSe
01637-07 ^a	Se LMM	1348.2	2.14	7.61x10 ³	CdSe
01637-08 ^a	Se LMM + C 1s	1202.1	1.54	4.29x10 ³	CdSe + Contaminant
01637-08 ^a	Se LMM	1190.4	3.38	3.80x10 ³	CdSe
01637-09	Cd 4d	10.9	1.42	3.54x10 ³	CdSe
01637-09 ^b	VBM	1.7	CdSe

^a Peak energy reported as kinetic energy (KE)

^b Valence band maximum (VBM)

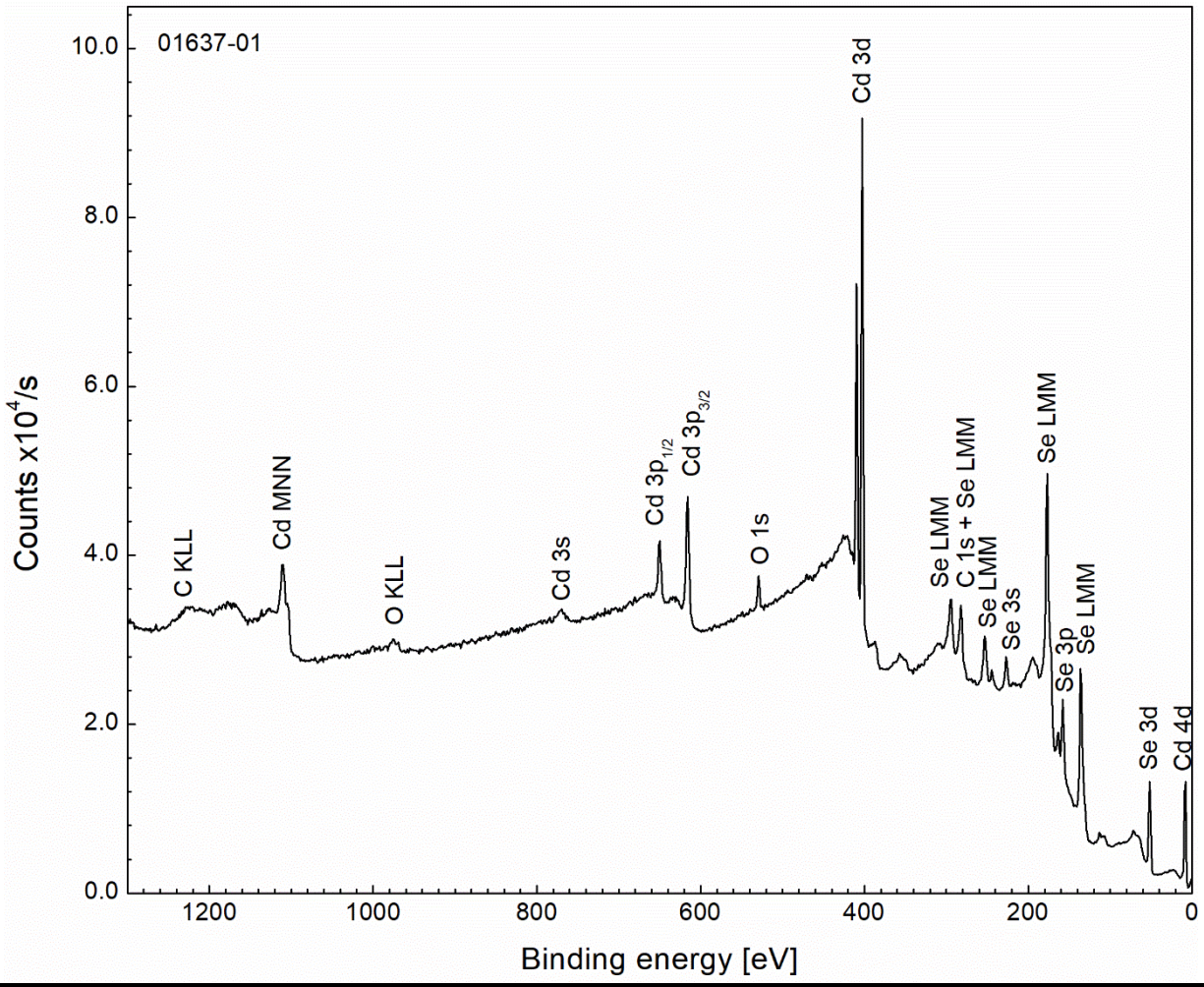
ANALYZER CALIBRATION TABLE							
Spectrum ID #	Element/ Transition	Peak Energy (eV)	Peak Width FWHM (eV)	Peak Area (eV x cts/s)	Sensitivity Factor	Concentration (at. %)	Peak Assignment
...	Ag 3d _{5/2}	368.3	0.50	0.15x10 ⁶

GUIDE TO FIGURES

Spectrum (Accession) #	Spectral Region	Voltage Shift*	Multiplier	Baseline	Comment #
01637-01	Survey	-	1	0	1
01637-02	Cd 3d	0.11	1	0	1
01637-03	Se 3d	0.11	1	0	1
01637-04	O 1s	0.11	1	0	1
01637-05	Cd 3p	0.11	1	0	1
01637-06	Cd MNN	0.11	1	0	1
01637-07	Se LMM, Se 3p	0.11	1	0	1
01637-08	Se LMM, C 1s	0.11	1	0	1
01637-09	Cd 4d, VB	0.11	1	0	1

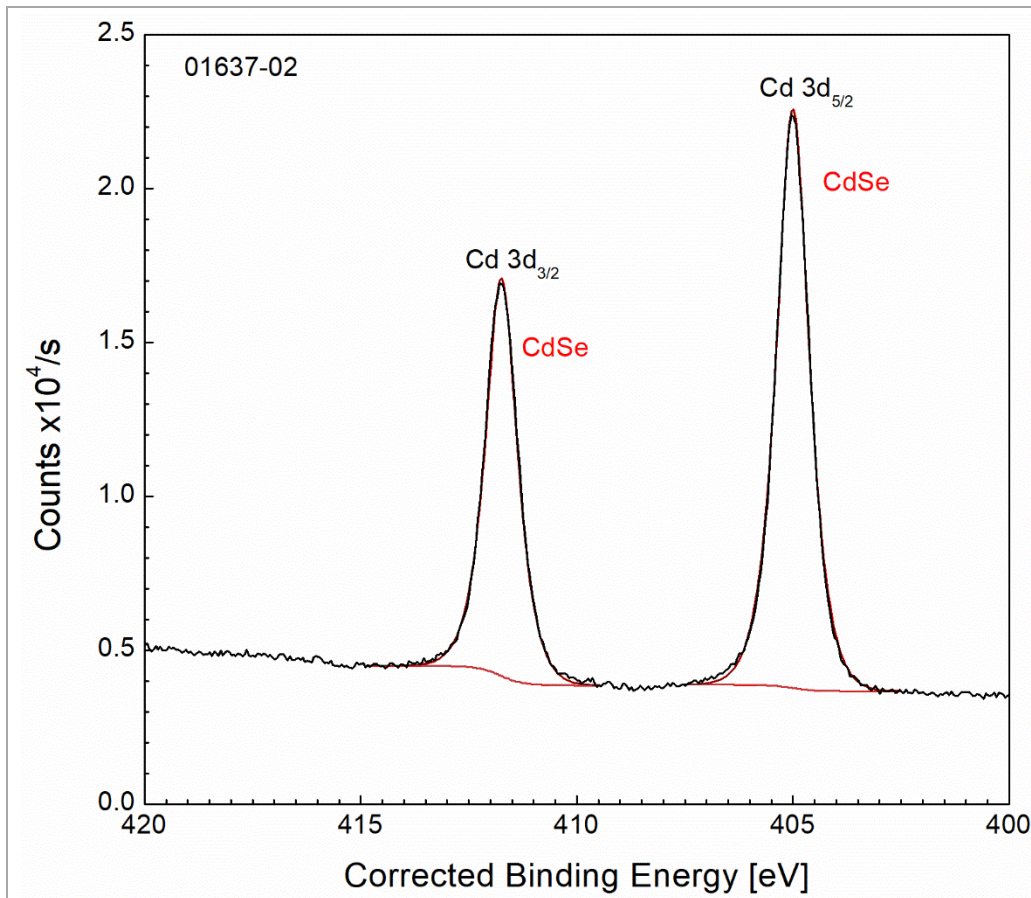
*Voltage shift of the archived (as-measured) spectrum relative to the printed figure. The figure reflects the recommended energy scale correction due to a calibration correction, sample charging, flood gun, or other phenomenon.

1. CdSe powder



Publish in *Surface Science Spectra*: Yes No

Accession #	01637-01
Host Material	CdSe
Technique	XPS
Spectral Region	survey
Instrument	SPECS PHOIBOS 150
Excitation Source	Al Ka monochromatic
Source Energy	1486.6 eV
Source Strength	200 W
Source Size	2 mm x 2 mm
Analyzer Type	spherical sector analyzer
Incident Angle	55°
Emission Angle	0°
Analyzer Pass Energy	100 eV
Analyzer Resolution	0.5 eV
Total Signal Accumulation Time	122 s
Total Elapsed Time	260 s
Number of Scans	1
Effective Detector Width	5.28 eV



Publish in SSS: Yes No

■ Accession #: 01637-02

■ Host Material: CdSe

■ Technique: XPS

■ Spectral Region: Cd 3d

Instrument: SPECS PHOIBOS 150

Excitation Source: Al Ka
monochromatic

Source Energy: 1486.6 eV

Source Strength: 200 W

Source Size: 2 mm x 2 mm

Analyzer Type: spherical sector

Incident Angle: 55 °

Emission Angle: 0 °

Analyzer Pass Energy 30 eV

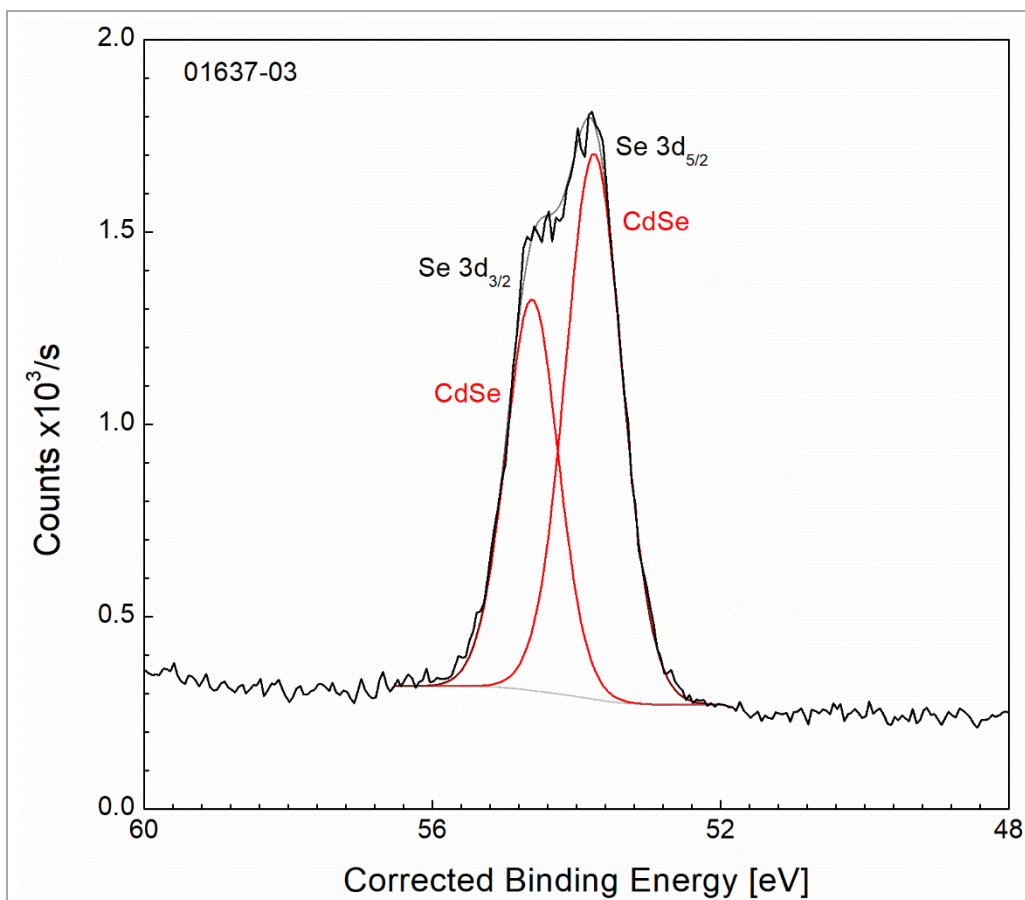
Analyzer Resolution: 0.5 eV

Total Signal Accumulation Time: 432
s

Total Elapsed Time: 720 s

Number of Scans: 8

Effective Detector Width: 2.64 eV



Publish in SSS: Yes No

■ Accession #: 01637-03

■ Host Material: CdSe

■ Technique: XPS

■ Spectral Region: Se 3d

Instrument: SPECS PHOIBOS 150

Excitation Source: Al Ka
monochromatic

Source Energy: 1486.6 eV

Source Strength: 200 W

Source Size: 2 mm x 2 mm

Analyzer Type: spherical sector

Incident Angle: 55 °

Emission Angle: 0 °

Analyzer Pass Energy 30 eV

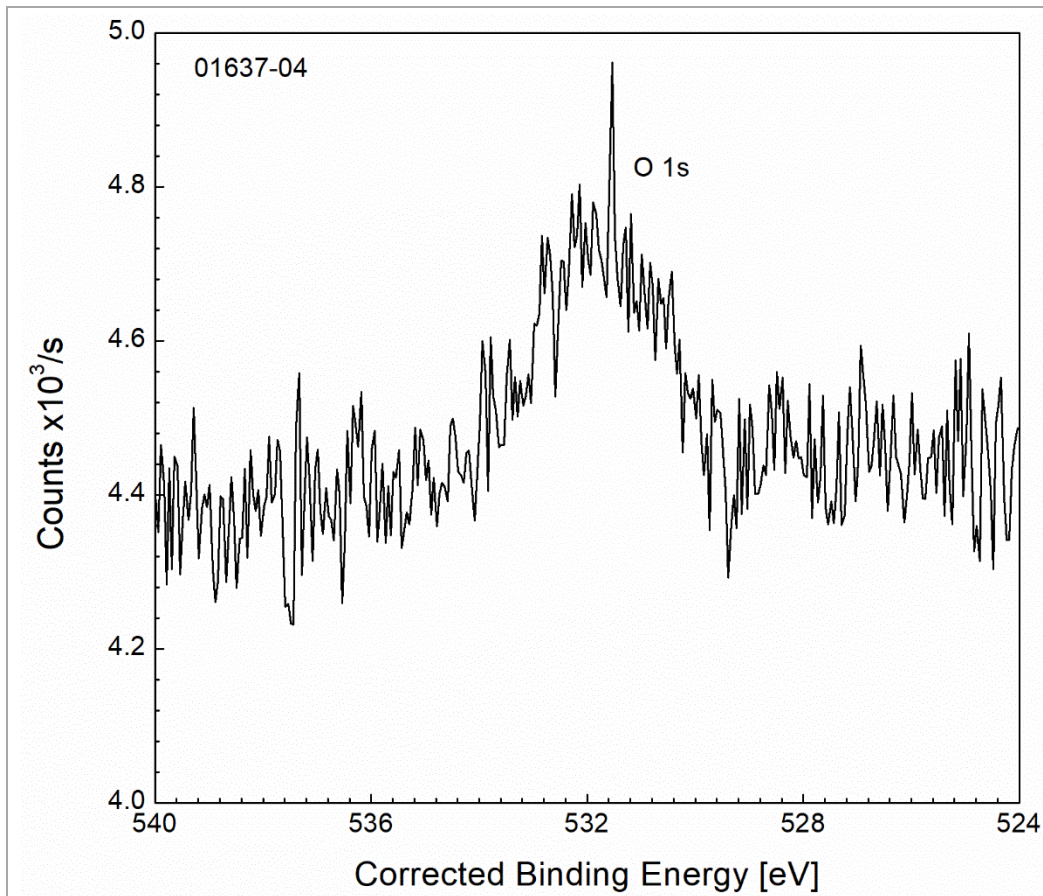
Analyzer Resolution: 0.5 eV

Total Signal Accumulation Time: 225 s

Total Elapsed Time: 420 s

Number of Scans: 8

Effective Detector Width: 2.64 eV



Publish in SSS: Yes No

■ Accession #: 01637-04

■ Host Material: CdSe

■ Technique: XPS

■ Spectral Region: O 1s

Instrument: SPECS PHOIBOS 150

Excitation Source: Al Ka
monochromatic

Source Energy: 1486.6 eV

Source Strength: 200 W

Source Size: 2 mm x 2 mm

Analyzer Type: spherical sector

Incident Angle: 55 °

Emission Angle: 0 °

Analyzer Pass Energy 30 eV

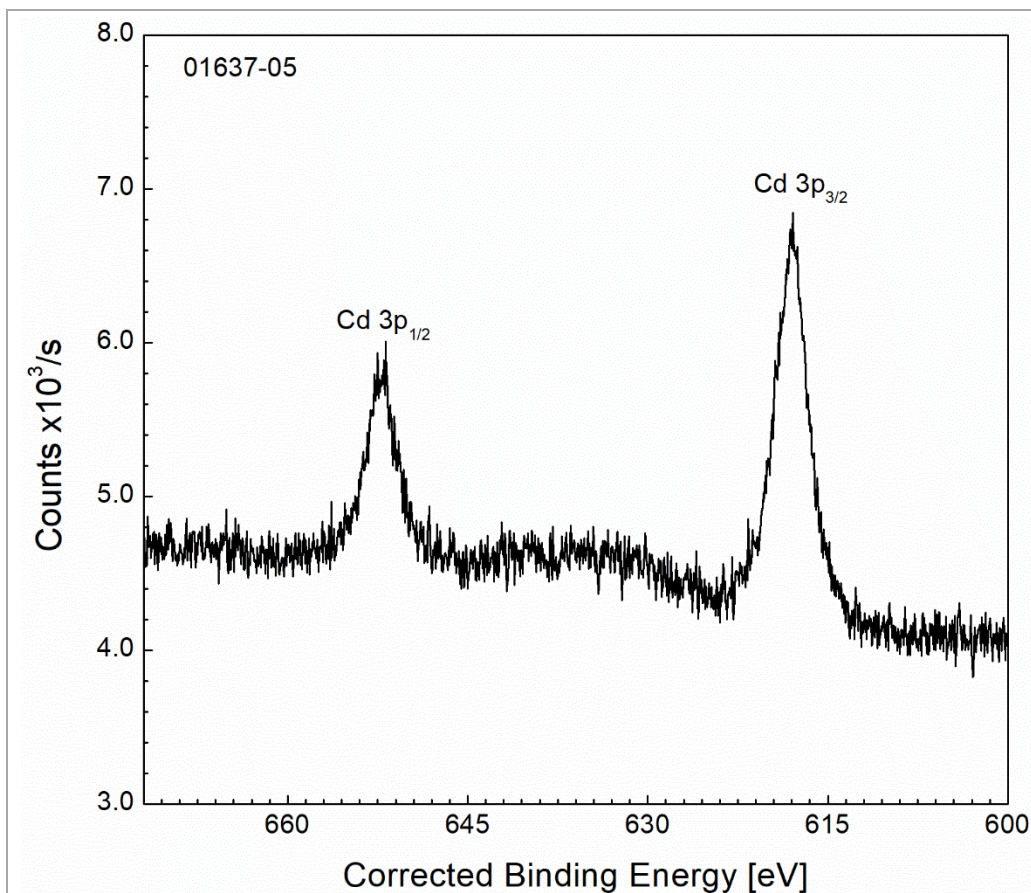
Analyzer Resolution: 0.5 eV

Total Signal Accumulation Time: 337
s

Total Elapsed Time: 564 s

Number of Scans: 8

Effective Detector Width: 2.64 eV



Publish in SSS: Yes No

■ Accession #: 01637-05

■ Host Material: CdSe

■ Technique: XPS

■ Spectral Region: Cd 3p

Instrument: SPECS PHOIBOS 150

Excitation Source: Al Ka
monochromatic

Source Energy: 1486.6 eV

Source Strength: 200 W

Source Size: 2 mm x 2 mm

Analyzer Type: spherical sector

Incident Angle: 55 °

Emission Angle: 0 °

Analyzer Pass Energy 30 eV

Analyzer Resolution: 0.5 eV

Total Signal Accumulation Time: 600
s

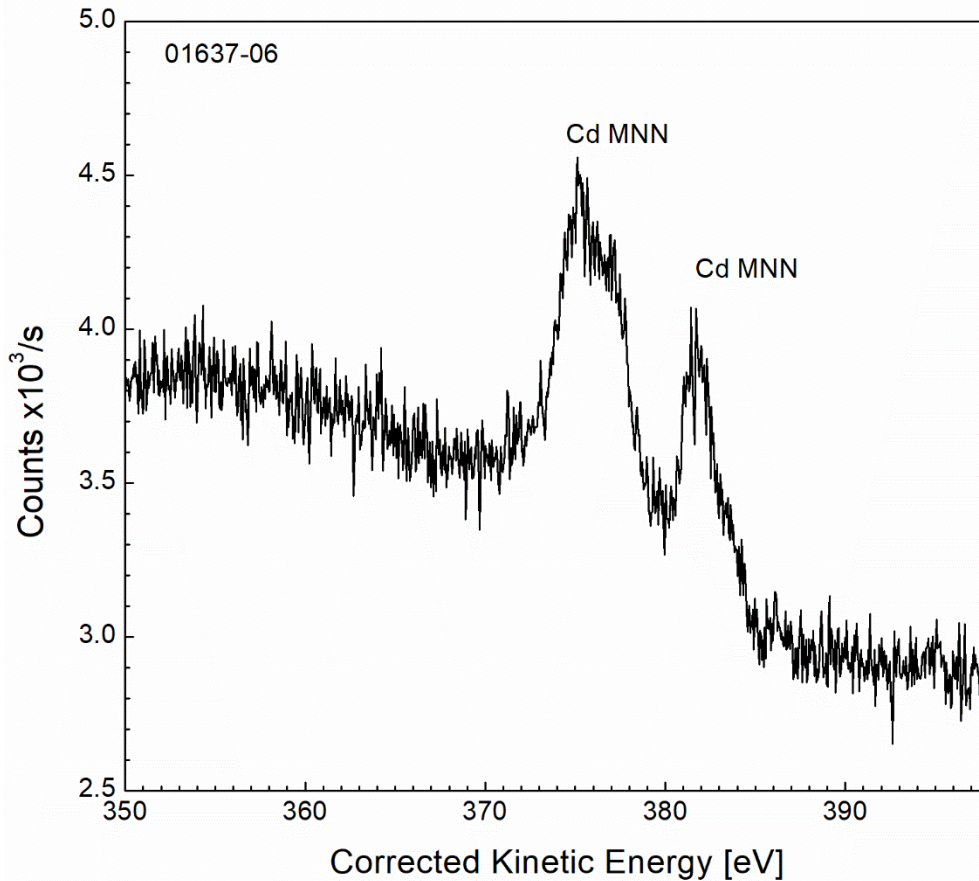
Total Elapsed Time: 913 s

Number of Scans: 4

Effective Detector Width: 2.64 eV

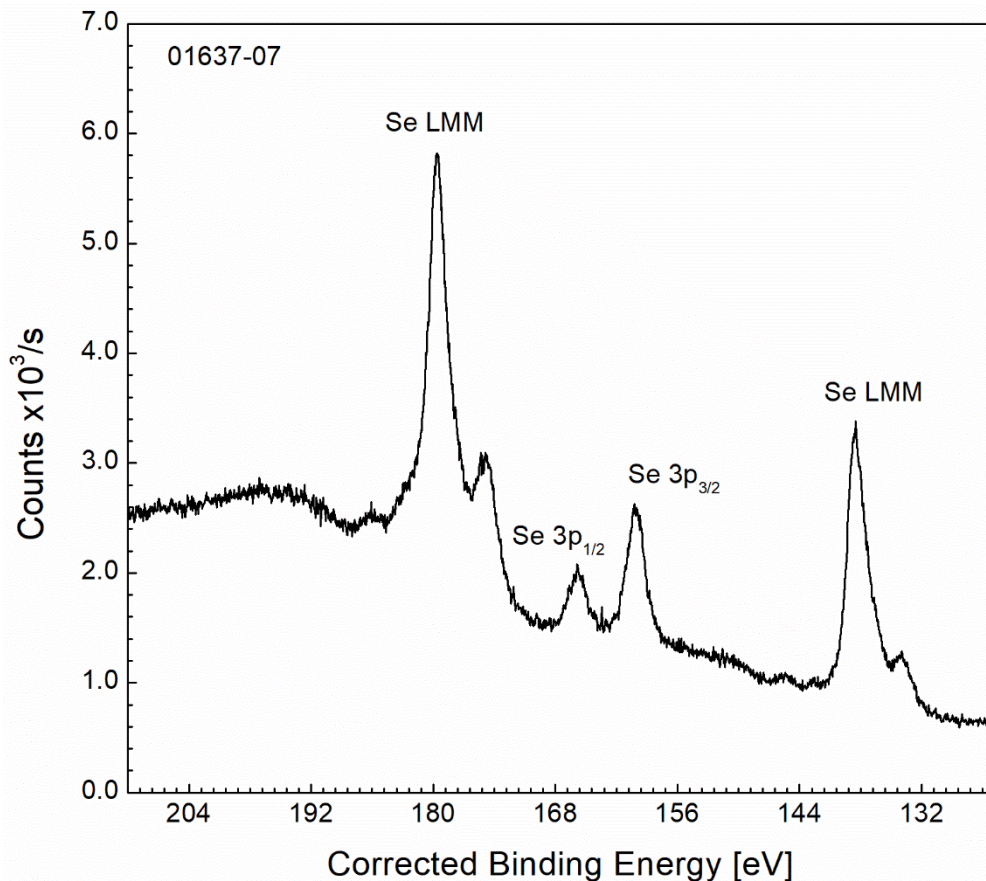
Publish in SSS: Yes No

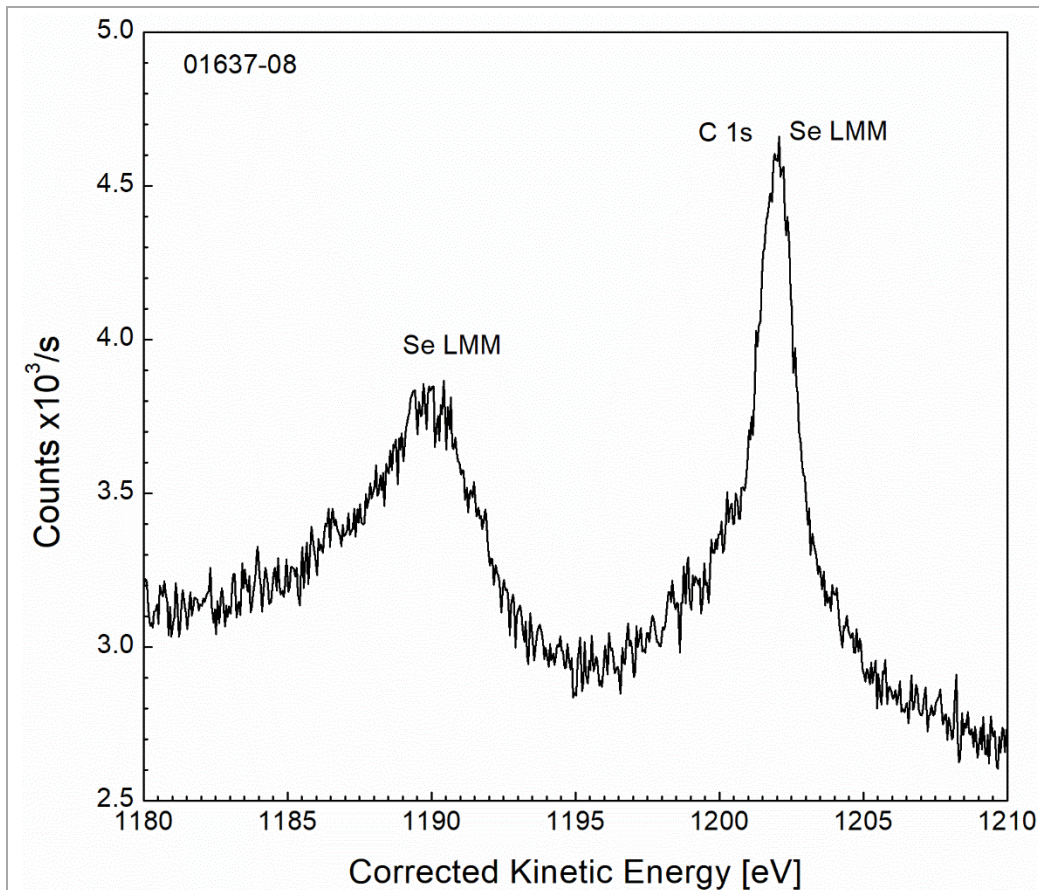
■ Accession #: 01637-06
■ Host Material: CdSe
■ Technique: XAES
■ Spectral Region: Cd MNN
Instrument: SPECS PHOIBOS 150
Excitation Source: Al Ka monochromatic
Source Energy: 1486.6 eV
Source Strength: 200 W
Source Size: 2 mm x 2 mm
Analyzer Type: spherical sector
Incident Angle: 55 °
Emission Angle: 0 °
Analyzer Pass Energy 30 eV
Analyzer Resolution: 0.5 eV
Total Signal Accumulation Time: 496 s
Total Elapsed Time: 764 s
Number of Scans: 4
Effective Detector Width: 2.64 eV



Publish in SSS: Yes No

■ Accession #: 01637-07
■ Host Material: CdSe
■ Technique: XPS, XAES
■ Spectral Region: Se LMM, Se 3p
Instrument: SPECS PHOIBOS 150
Excitation Source: Al Ka monochromatic
Source Energy: 1486.6 eV
Source Strength: 200 W
Source Size: 2 mm x 2 mm
Analyzer Type: spherical sector
Incident Angle: 55 °
Emission Angle: 0 °
Analyzer Pass Energy 30 eV
Analyzer Resolution: 0.5 eV
Total Signal Accumulation Time: 1489 s
Total Elapsed Time: 2244 s
Number of Scans: 8
Effective Detector Width: 2.64 eV





Publish in SSS: Yes No

■ Accession #: 01637-08

■ Host Material: CdSe

■ Technique: XAES

■ Spectral Region: C 1s, Se LMM

Instrument: SPECS PHOIBOS 150

Excitation Source: Al Ka
monochromatic

Source Energy: 1486.6 eV

Source Strength: 200 W

Source Size: 2 mm x 2 mm

Analyzer Type: spherical sector

Incident Angle: 55 °

Emission Angle: 0 °

Analyzer Pass Energy 30 eV

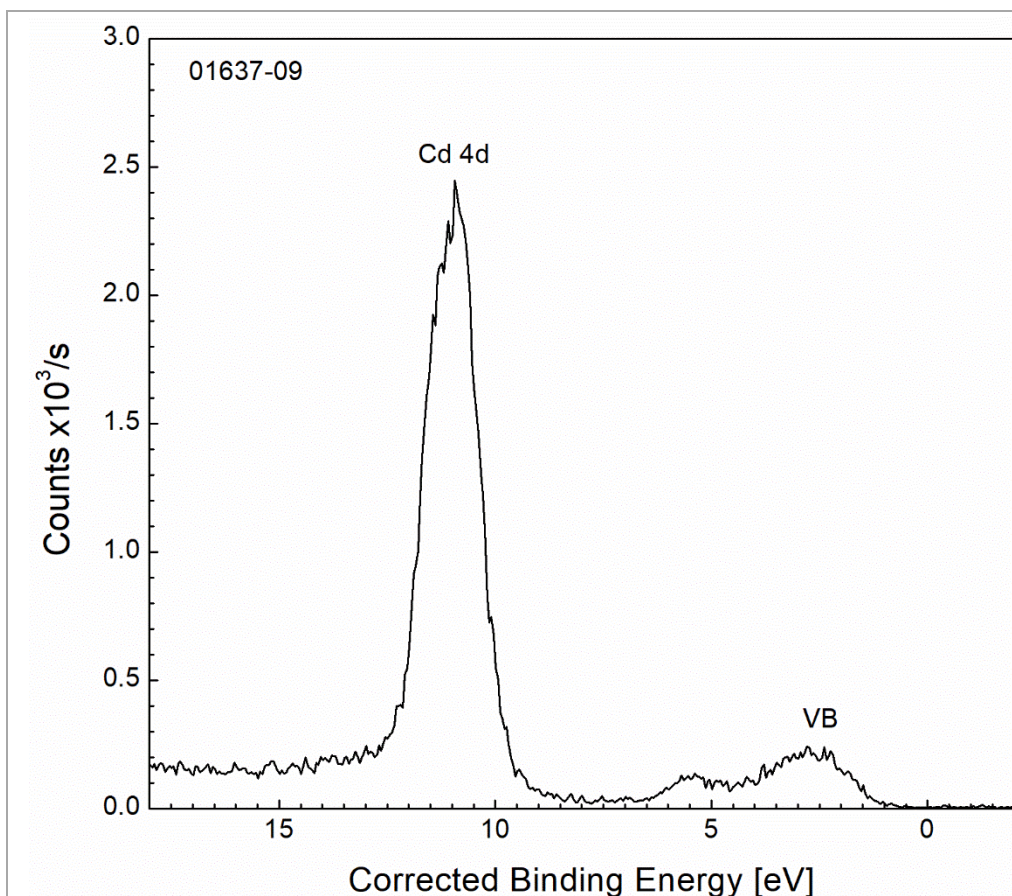
Analyzer Resolution: 0.5 eV

Total Signal Accumulation Time: 544
s

Total Elapsed Time: 876 s

Number of Scans: 8

Effective Detector Width: 2.64 eV



Publish in SSS: Yes No

■ Accession #: 01637-09

■ Host Material: CdSe

■ Technique: XPS

■ Spectral Region: Cd 4d, VB

Instrument: SPECS PHOIBOS 150

Excitation Source: Al Ka
monochromatic

Source Energy: 1486.6 eV

Source Strength: 200 W

Source Size: 2 mm x 2 mm

Analyzer Type: spherical sector

Incident Angle: 55 °

Emission Angle: 0 °

Analyzer Pass Energy 30 eV

Analyzer Resolution: 0.5 eV

Total Signal Accumulation Time: 304 s

Total Elapsed Time: 485 s

Number of Scans: 4

Effective Detector Width: 2.64 eV