**Cadmium selenide by XPS**

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(Received day Month year; accepted day Month year; published day Month year)

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

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**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=EN):** N=0

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

- **Excitation Source:** Al Ka monochromatic

- **Source Energy:** 1486.6 eV

- **Source Strength:** 200 W

- **Source Beam Size:** 2000 µm x 2000 µm

- **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

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**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 x 10⁻⁷ Pa

**Pre-analysis Beam Exposure:** Not applicable s

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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 3d₅/₂ = 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

Authors thank to Laboratorio Central en Ciencia de Superficies (SurLab-UIS) from Universidad Industrial de Santander for providing their facilities to perform the XPS measurements and to project 2321 of Vicerrectoría de Investigación y Extensión (VIE-UIS) from Universidad Industrial de Santander.

REFERENCES

### SPECTRAL FEATURES TABLE

<table>
<thead>
<tr>
<th>Spectrum ID #</th>
<th>Element/Transition</th>
<th>Peak Energy (eV)</th>
<th>Peak Width FWHM (eV)</th>
<th>Peak Area (eV x cts/s)</th>
<th>Sensitivity Factor</th>
<th>Concentration (at. %)</th>
<th>Peak Assignment</th>
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<tbody>
<tr>
<td>01637-02</td>
<td>Cd 3d</td>
<td>...</td>
<td>...</td>
<td>1.94x10^4</td>
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<td>O 1s</td>
<td>531.5</td>
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<tr>
<td>01637-06a</td>
<td>Cd MNN</td>
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* Peak energy reported as kinetic energy (KE)
* Valence band maximum (VBM)

### ANALYZER CALIBRATION TABLE

<table>
<thead>
<tr>
<th>Spectrum ID #</th>
<th>Element/Transition</th>
<th>Peak Energy (eV)</th>
<th>Peak Width FWHM (eV)</th>
<th>Peak Area (eV x cts/s)</th>
<th>Sensitivity Factor</th>
<th>Concentration (at. %)</th>
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<tr>
<td>...</td>
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<td>Spectrum (Accession) #</td>
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<td>Baseline</td>
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<td>1</td>
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*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
<table>
<thead>
<tr>
<th>Accession #</th>
<th>01637-01</th>
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<tbody>
<tr>
<td>Host Material</td>
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<tr>
<td>Technique</td>
<td>XPS</td>
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<td>Spectral Region</td>
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<tr>
<td>Instrument</td>
<td>SPECS PHOIBOS 150</td>
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<tr>
<td>Excitation Source</td>
<td>Al Ka monochromatic</td>
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<tr>
<td>Source Energy</td>
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</tr>
<tr>
<td>Source Strength</td>
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</tr>
<tr>
<td>Source Size</td>
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<tr>
<td>Analyzer Type</td>
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<tr>
<td>Incident Angle</td>
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<tr>
<td>Emission Angle</td>
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<tr>
<td>Analyzer Pass Energy</td>
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<td>Analyzer Resolution</td>
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<tr>
<td>Total Signal Accumulation Time</td>
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<td>Total Elapsed Time</td>
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<tr>
<td>Number of Scans</td>
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<tr>
<td>Effective Detector Width</td>
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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

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
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

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
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

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
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

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