

Supporting Information

Ternary Cu₂SnS₃: Synthesis, Structure, Photoelectrochemical Activity, and Heterojunction Band Offset and Alignment

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The Supporting Information contains 14 Figures (three possible model arrangement of Cu and Sn ions at the 4a sites in CTS; partial density of states (PDOS) of CTS models; crystal structure, PDOS, band structure and effective masses of ZnS and CdS; geometry optimized surface model of CTS(111), CdS(100), and ZnS(110) surfaces used to align the electronic eigenvalues to the vacuum level; EDX spectra and elemental mapping of CTS NPs; SEM images of CTS NPs; chronoamperometry photocurrent stability test for the CTS thin film under illumination of the AM1.5G solar light; X-ray diffraction pattern, Raman spectrum and UV-vis absorbance spectra of CdS and ZnS NPs; and photoanodic behaviour of CdS and ZnS NPs). The relaxed structures with the lattice parameters and atomic positions for the bulk structures, and for the surface slabs generated are also given.

Figure S1: Three possible arrangement of Cu and Sn ions at the 4a sites in CTS: (a) Model-1, (b) Model-2, and (c) Model-3. Model-1 is energetically more favourable than Model-2 by 4.54 eV and Model-3 by 11.98 eV. Atomic color: Cu =brown, Sn =pink and S =yellow.

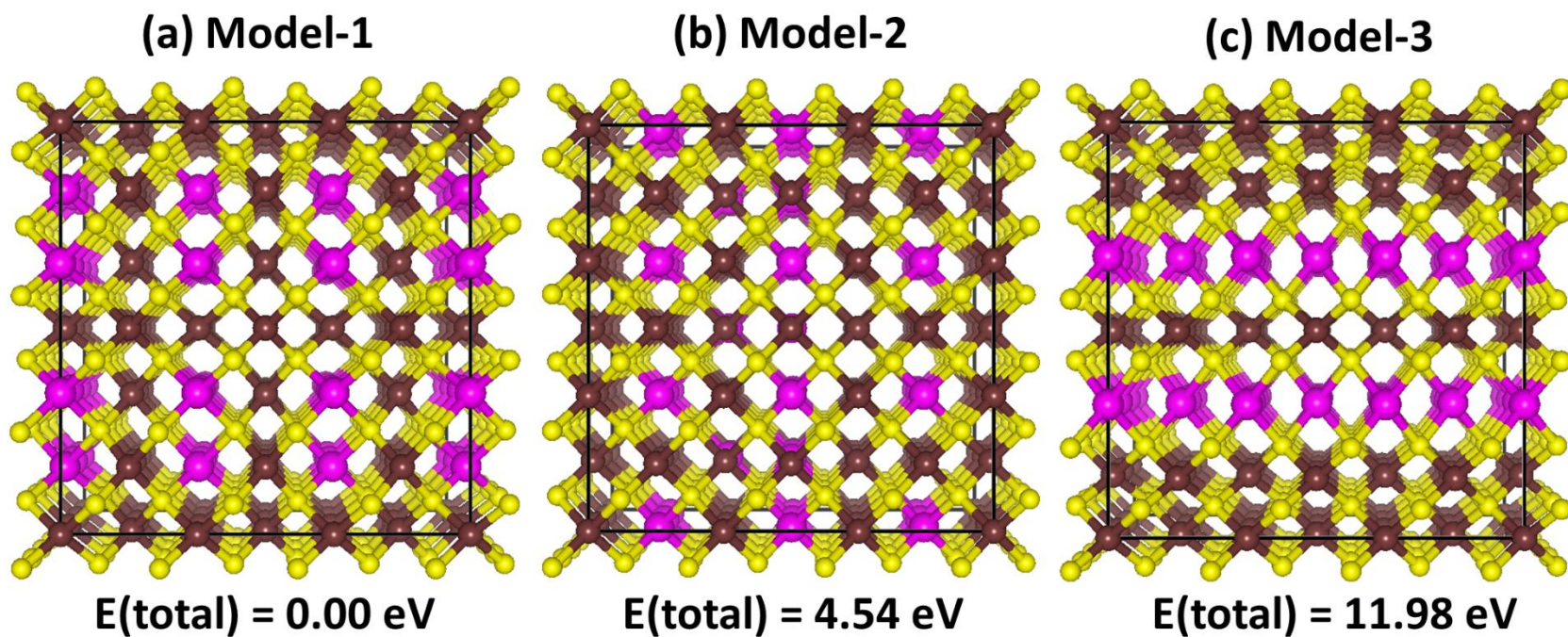


Figure S2: The partial density of states of CTS in (a) Model-1, (b) Model-2, and (c) Model-3.

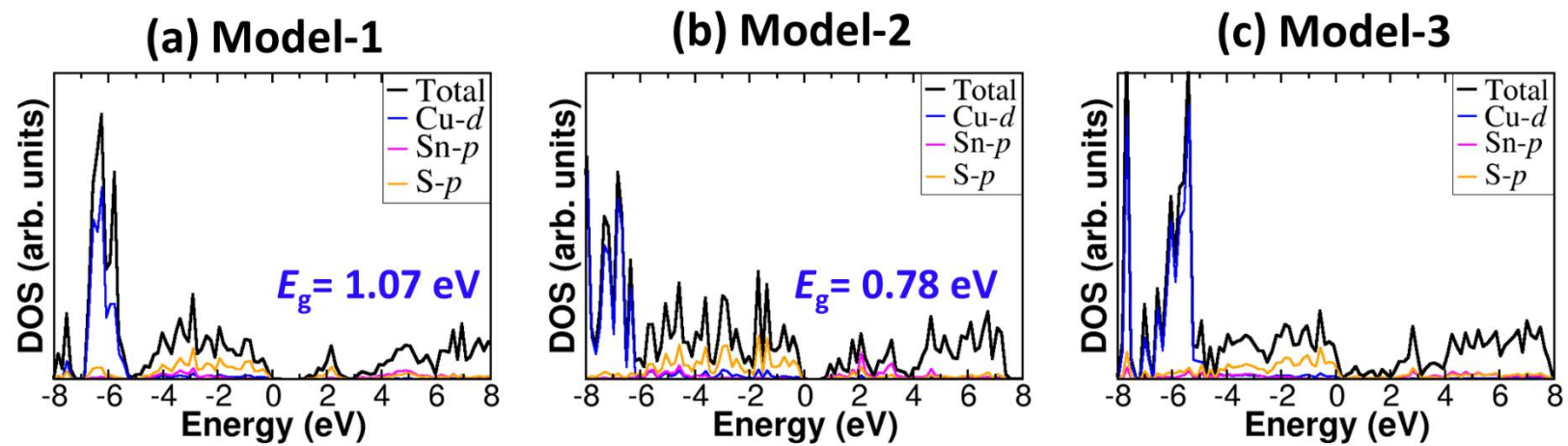


Figure S3: (a) Crystal structure, (b) partial density of states (PDOS), and (c) band structure of ZnS. The calculated corresponding effective masses of holes and electrons along the high-symmetry directions of the Brillouin zone are shown in (d). Atomic color: Zn =grey, and S =yellow.

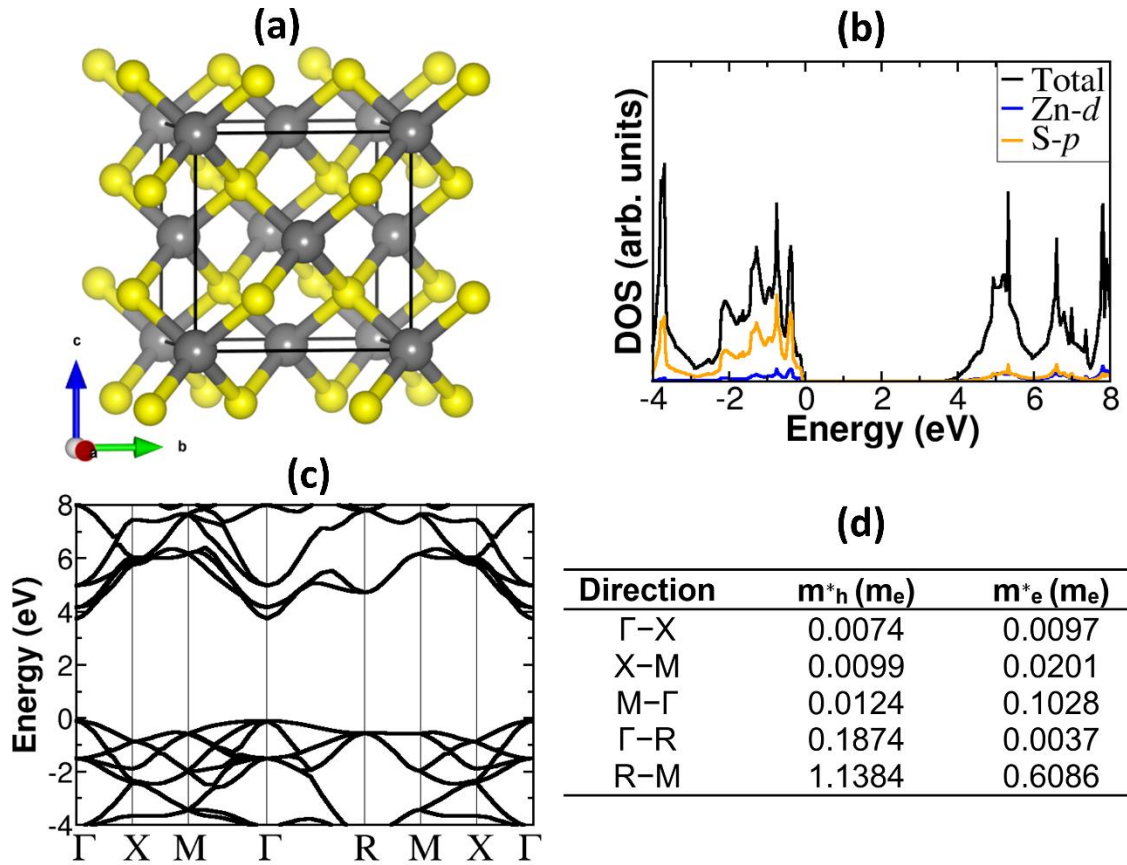


Figure S4: (a) Crystal structure, (b) partial density of states (PDOS), and (c) band structure of CdS. The calculated corresponding effective masses of holes and electrons along the high-symmetry directions of the Brillouin zone are shown in (d). Atomic color: Cd =black, and S =yellow.

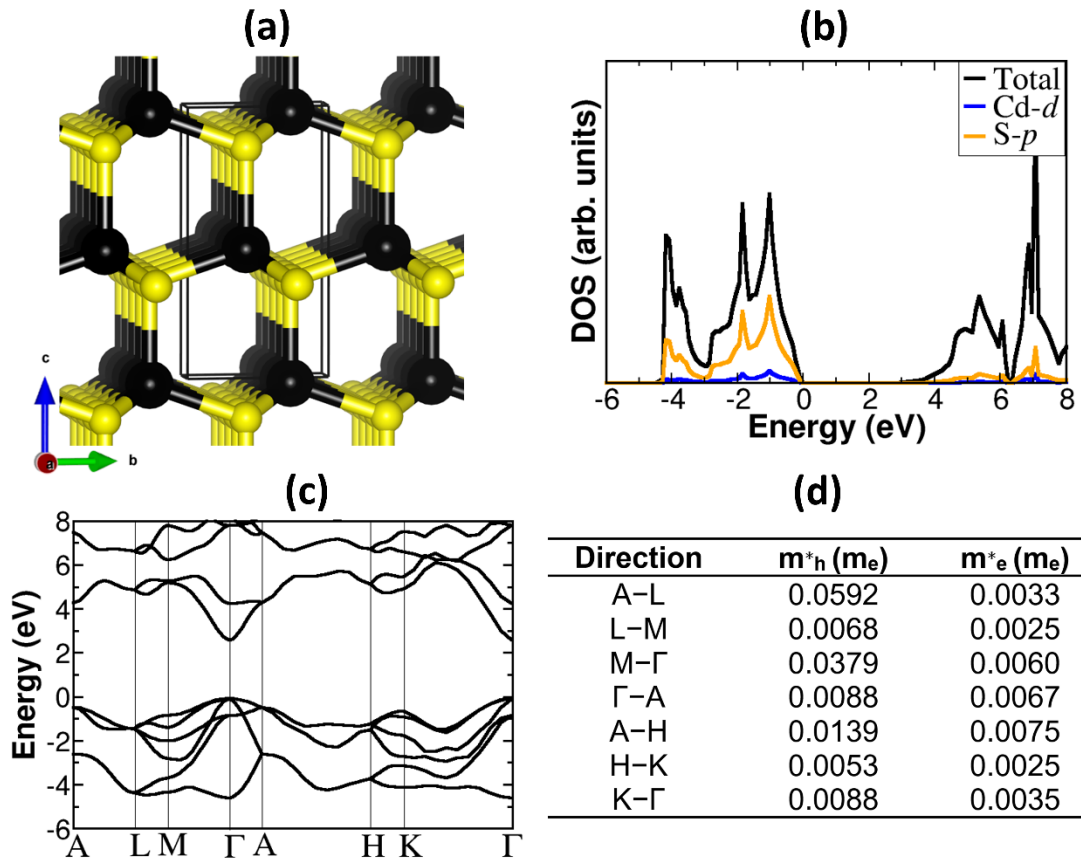


Figure S5: Geometry optimized model of the CTS(111) surface used to align the electronic eigenvalues to the vacuum level. The corresponding electrostatic potential is shown in blue.

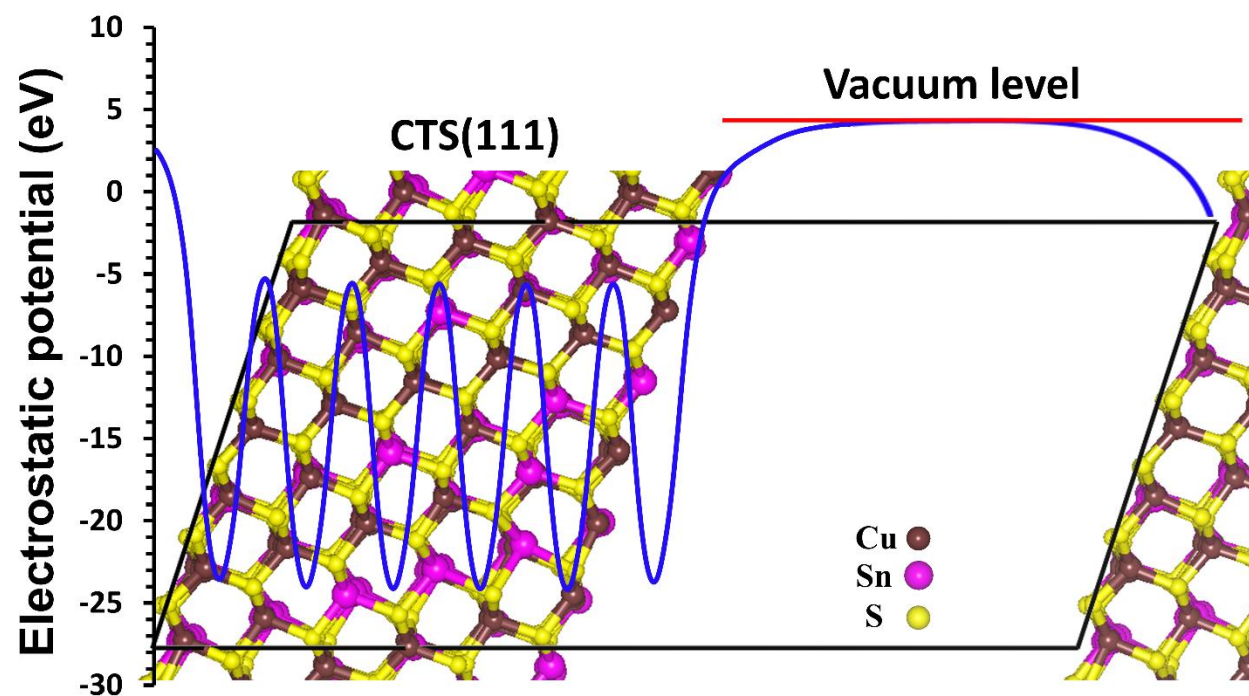


Figure S6: Geometry optimized model of the CdS(100) surface used to align the electronic eigenvalues to the vacuum level. The corresponding electrostatic potential is shown in blue.

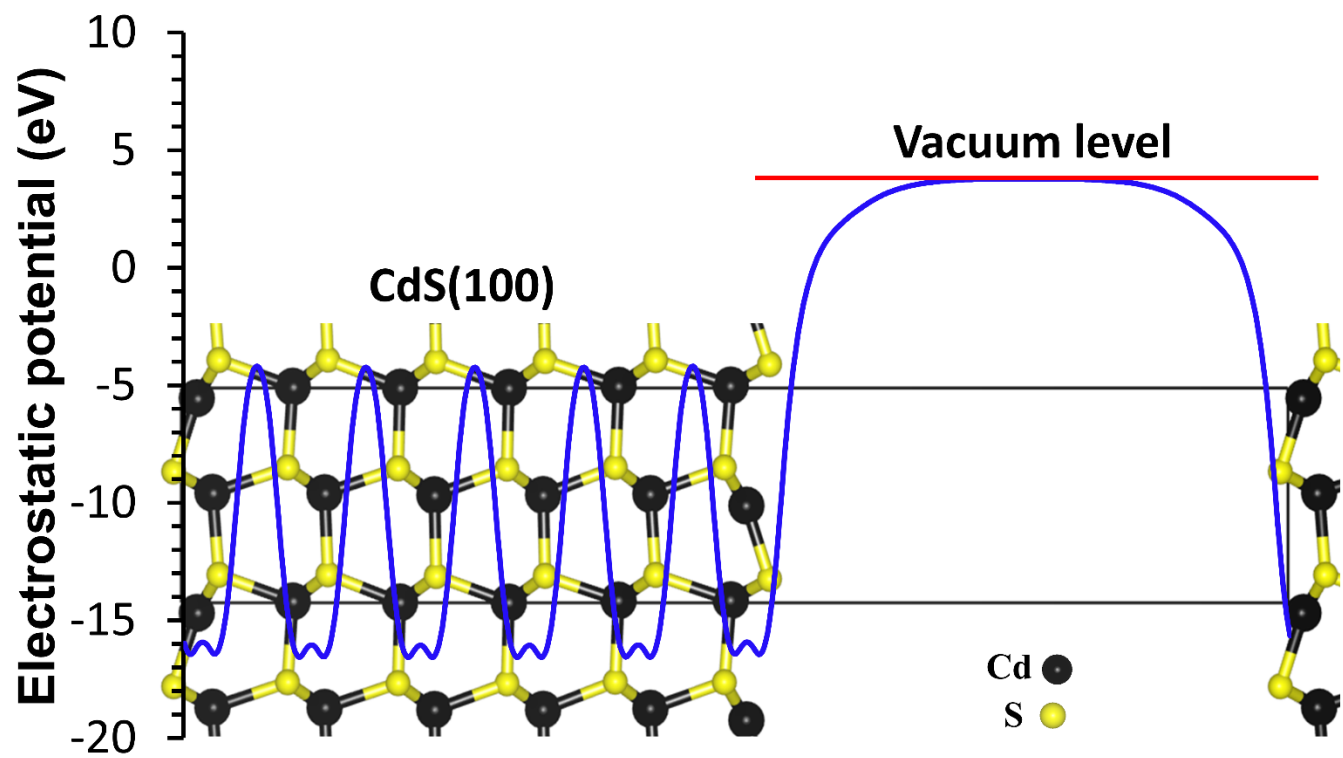


Figure S7: Geometry optimized model of the ZnS(110) surface used to align the electronic eigenvalues to the vacuum level. The corresponding electrostatic potential is shown in blue.

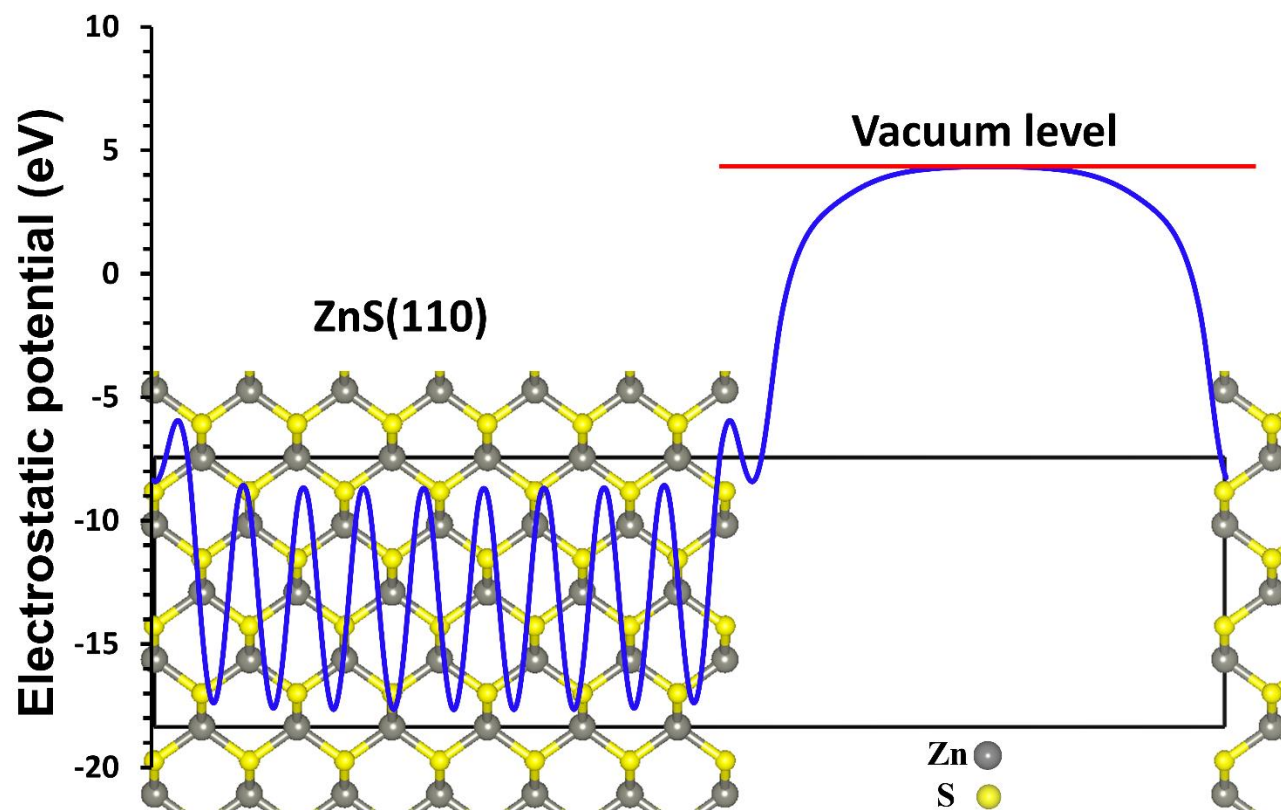


Figure S8: (a) EDX spectra of CTS NPs (c, d, e) Elemental mapping of Cu, Sn and S, respectively

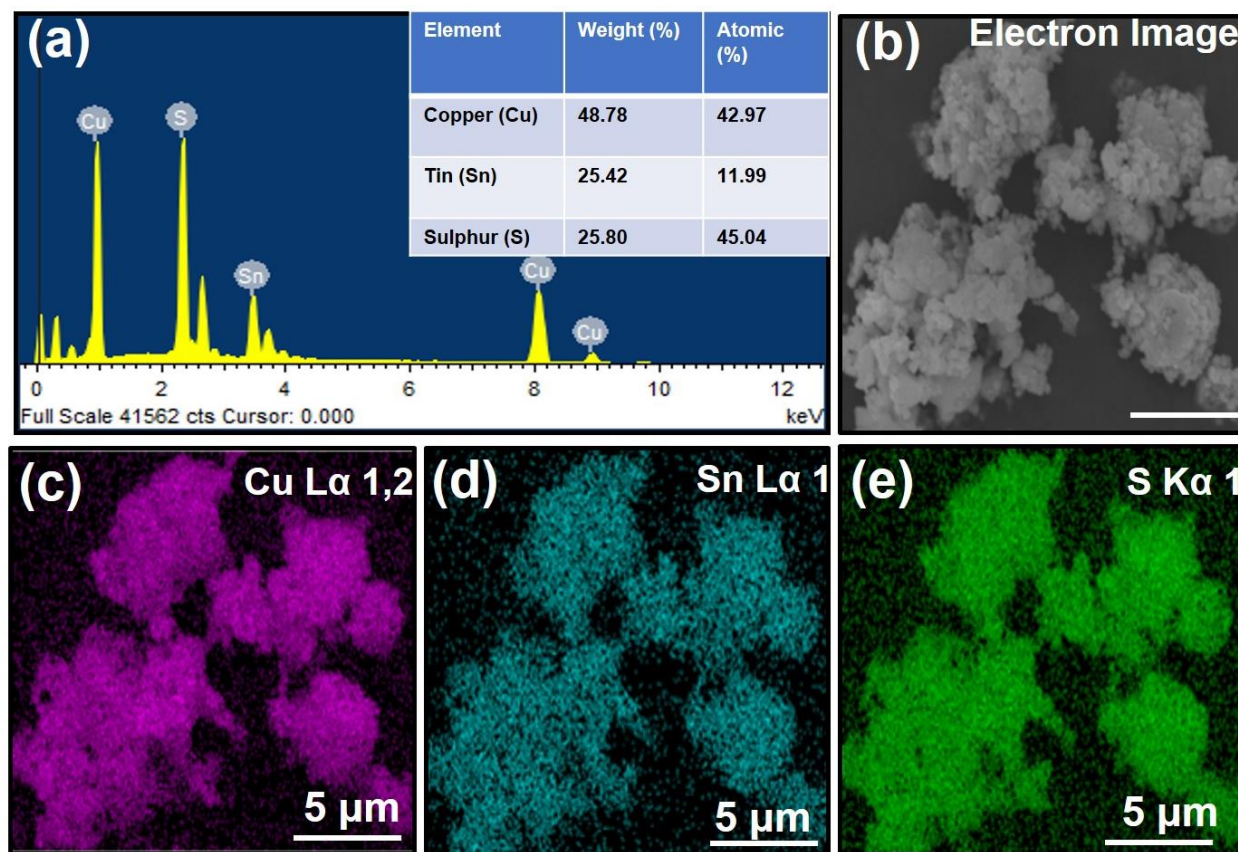


Figure S9: (a, b) SEM images of CTS NPs sample at different magnification

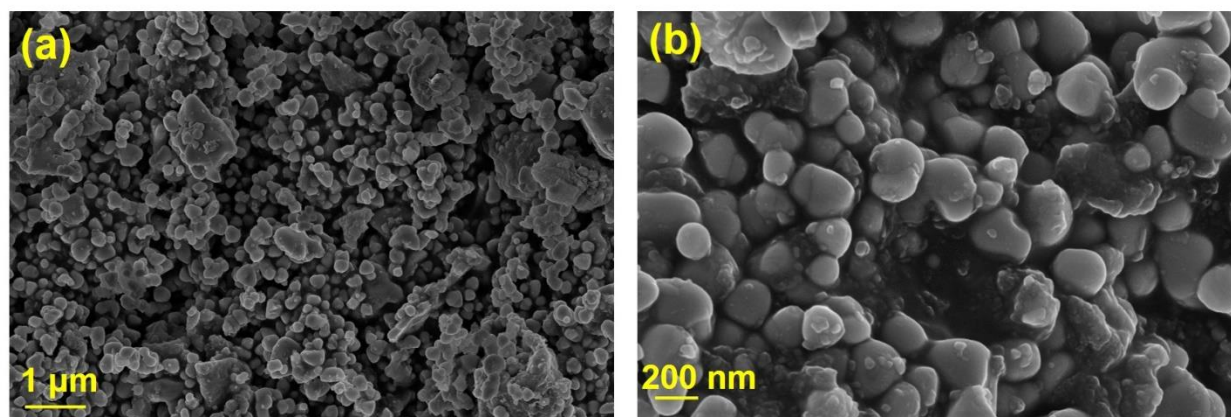


Figure S10: Chronoamperometry photocurrent stability test for the CTS thin film under illumination of the AM1.5G solar light.

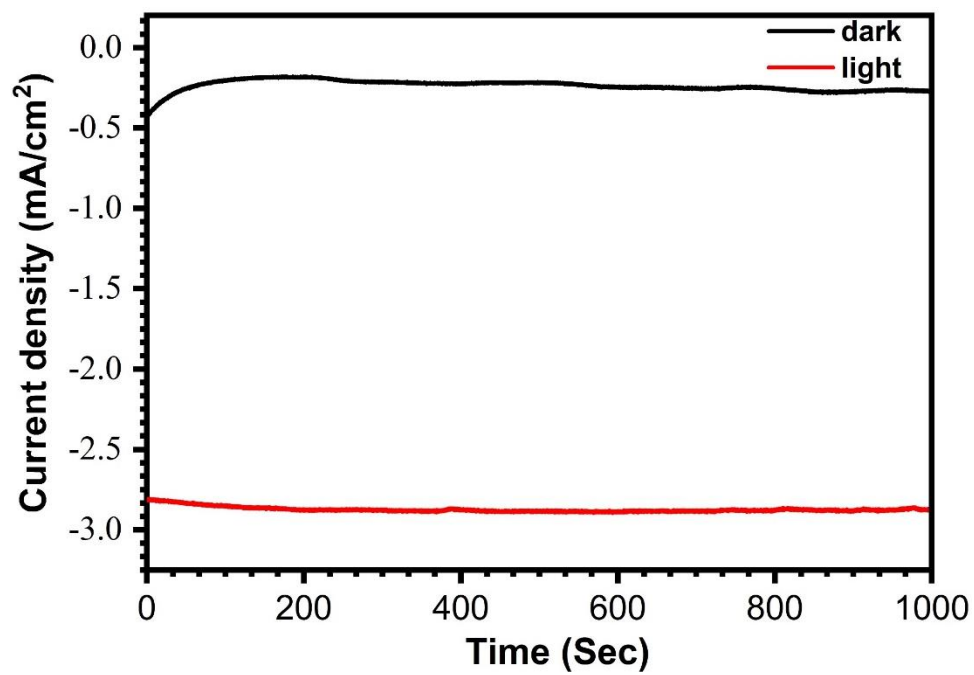


Figure S11: (a) X-ray diffraction pattern of CdS NPs. (b) Raman spectrum of CdS NPs. (c) UV-visible absorbance spectra of CdS NPs (d) band gap (Tauc) plot of CdS NPs.

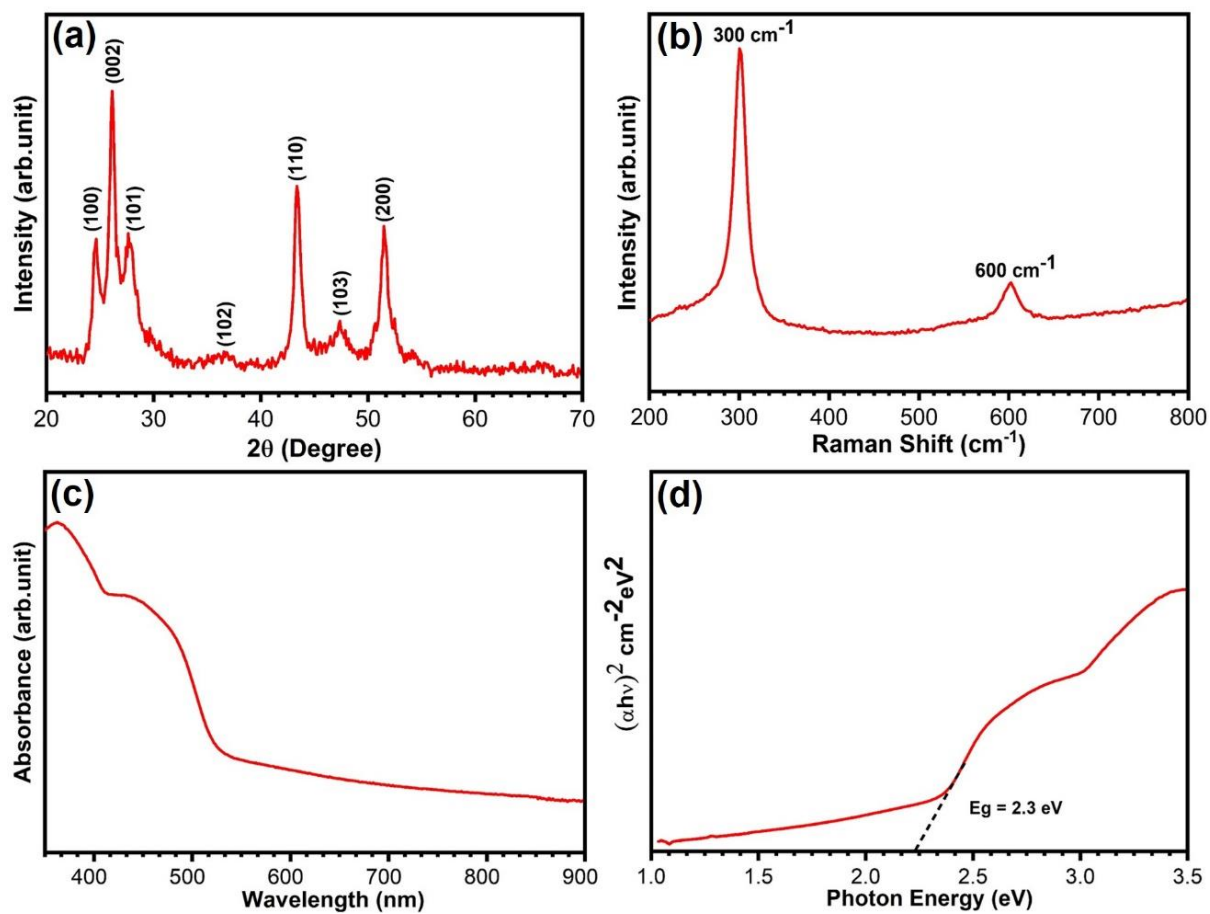


Figure S12: (a) XRD pattern of ZnS NPs synthesized by hot injection method. (b) FTIR spectra of ZnS NPs (c) UV-vis absorbance spectra of ZnS NPs. (d) Band gap plot of ZnS NPs

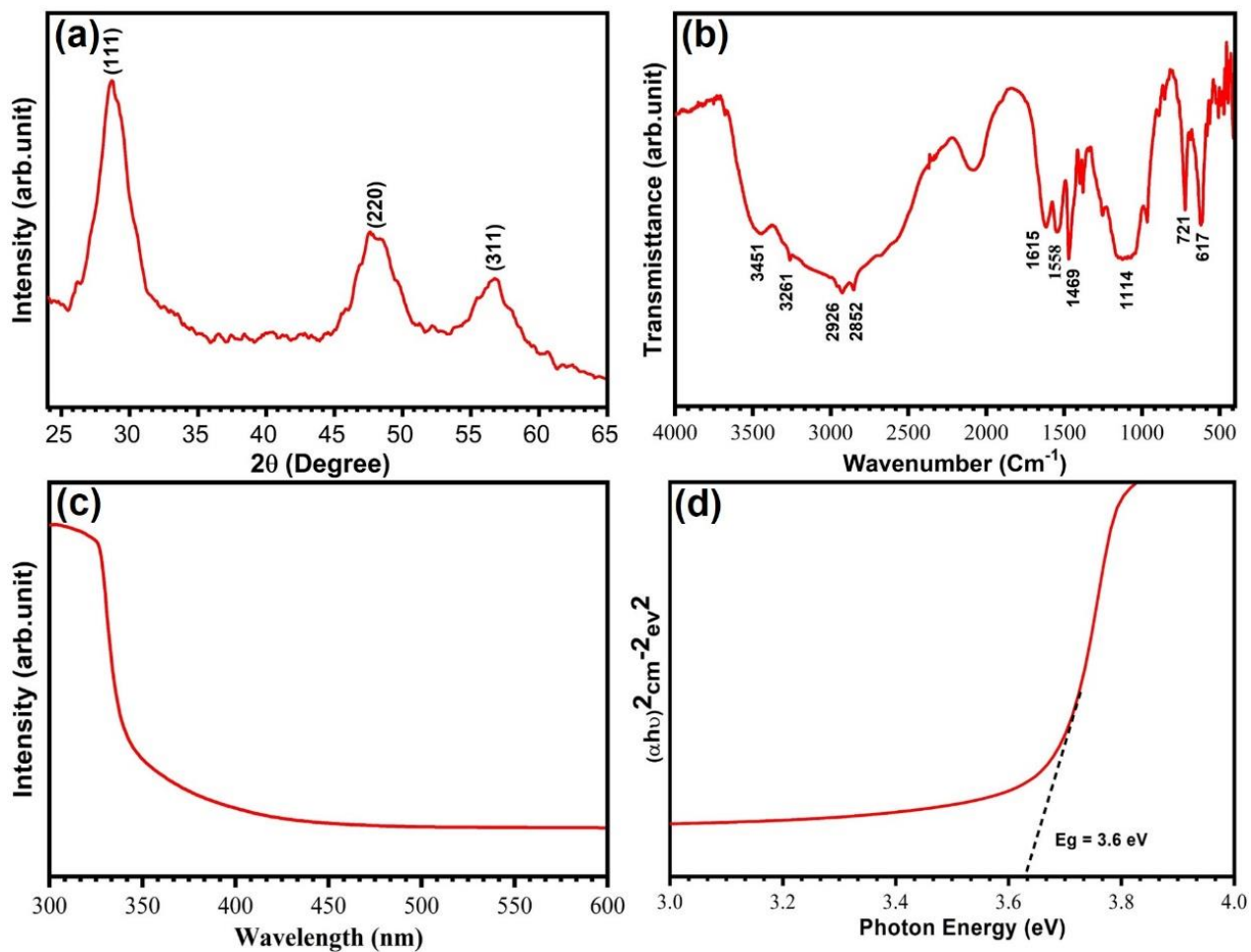


Figure S13: (a) Bode phase plot. (b) Z' real vs. $-Z''$ imaginary impedance plot (Nyquist plot) of CdS. (c) Mott-Schottky plot. (d) Current Density-Potential curves of CdS under simulated AM 1.5 G light irradiation in different conditions.

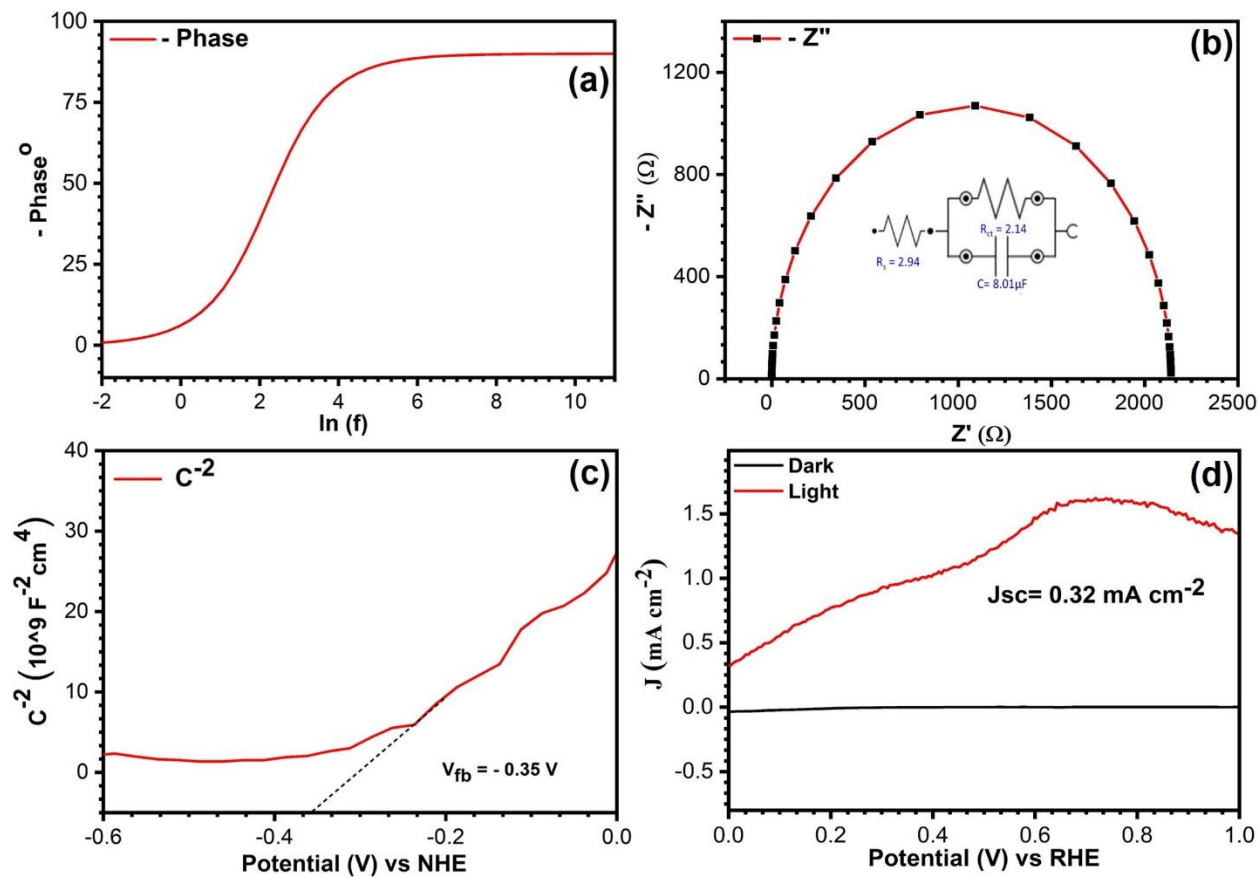
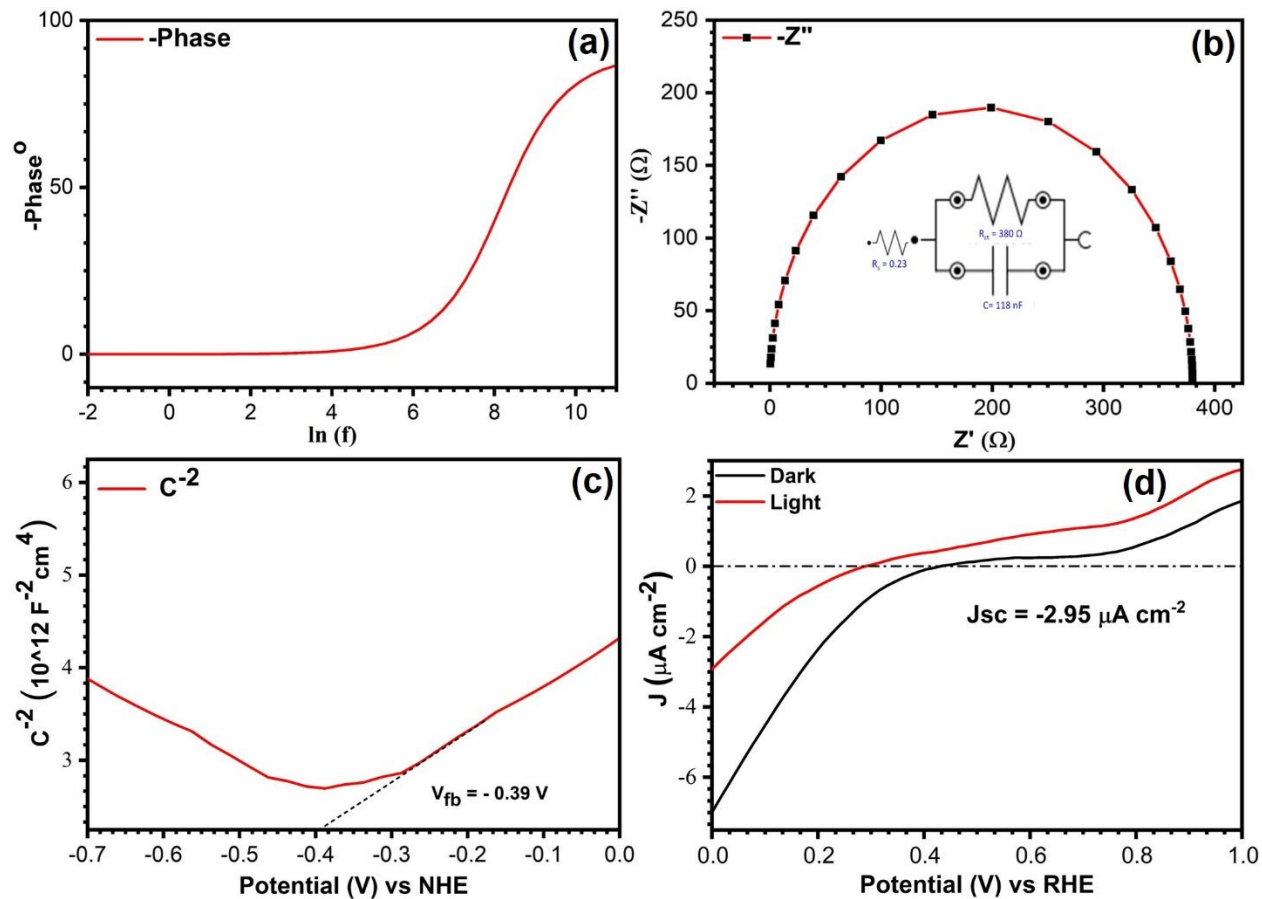


Figure S14: (a) Bode Phase plot. (b) Z' real vs. $-Z''$ imaginary impedance plot (Nyquist plot) of ZnS. (c) Mott-Schottky plot. (d) Current Density-Potential curves of ZnS under simulated AM 1.5 G light irradiation in different conditions.



Bulk CTS: Model-1 Structural parameters (VASP)

Cu Sn S

1.0000000000000000
16.2923717227231606 0.0000000000000000 0.0000000000000000
0.0000000000000000 16.2096464468226920 0.0000000000000000
0.0000000000000000 0.0000000000000000 16.2869151160225449

72 36 108

Cartesian

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0.0000000000	2.7016080000	13.6265290000
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14.9346740000	14.7155700000	12.2151860000
12.2192780000	12.3005080000	12.2151860000
12.1349930000	14.7690580000	15.0301110000

Bulk CTS: Model-2 Structural parameters (VASP)

Cu Sn S

1.0000000000000000
16.4319356750770709 0.0000000000000000 0.2187760184372871
0.0000000000000000 16.1000178401744414 0.0000000000000000
0.2167082976366084 0.0000000000000000 16.3079773495375697
72 36 108

Cartesian

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0.0361180000	2.5366600000	2.7179960000
2.8353280000	-0.0163350000	2.7022090000
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2.9075640000	-0.0163350000	8.1382020000
0.1444720000	-0.0195080000	10.8719850000
0.1805900000	2.5366600000	13.5899810000
2.9798000000	-0.0163350000	13.5741940000
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13.969139000	5.174823000	8.499679000
11.323588000	5.141134000	11.280441000
14.041375000	5.174823000	13.935671000
11.063002000	10.882654000	0.229126000
10.983957000	13.415868000	2.925905000
13.861988000	10.891479000	2.913171000
11.135238000	10.882654000	5.665119000
11.056193000	13.415868000	8.361897000
13.934224000	10.891479000	8.349163000
11.207475000	10.882654000	11.101110000
11.128429000	13.415868000	13.797890000
14.006460000	10.891479000	13.785155000
5.223773000	8.062057000	2.511388000
8.252087000	5.727318000	2.827384000
5.296010000	8.062057000	7.947381000
8.324323000	5.727318000	8.263377000
5.368246000	8.062057000	13.383373000
8.396559000	5.727318000	13.699369000
11.280398000	8.062057000	3.143381000
11.352635000	8.062057000	8.579373000
11.424871000	8.062057000	14.015366000
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2.767167000	2.553322000	5.398484000
2.839403000	2.553322000	10.834476000
2.437442000	8.024669000	-0.094540000
2.509678000	8.024669000	5.341453000
2.581914000	8.024669000	10.777445000
2.717501000	13.520158000	0.000854000
2.789737000	13.520158000	5.436847000
2.861974000	13.520158000	10.872839000
8.215968000	2.565820000	0.109388000
8.288204000	2.565820000	5.545381000
8.360440000	2.565820000	10.981374000
8.215968000	8.769123000	0.109388000
8.288204000	8.769123000	5.545381000
8.360440000	8.769123000	10.981374000
8.215968000	13.485186000	0.109388000
8.288204000	13.485186000	5.545381000
8.360440000	13.485186000	10.981374000
13.737006000	2.553322000	0.256285000
13.809242000	2.553322000	5.692277000
13.881478000	2.553322000	11.128270000
13.994495000	8.024669000	0.313316000
14.066731000	8.024669000	5.749309000
14.138968000	8.024669000	11.185301000
13.714435000	13.520158000	0.217922000
13.786671000	13.520158000	5.653914000
13.858907000	13.520158000	11.089907000
4.258662000	1.196904000	4.022135000
4.120943000	3.976083000	1.379627000
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1.310585000	3.952345000	3.996330000
4.330898000	1.196904000	9.458128000
4.193179000	3.976083000	6.815620000
1.403021000	1.164921000	6.871442000

1.3828210000	3.9523450000	9.4323230000
4.4031340000	1.1969040000	14.8941200000
4.2654150000	3.9760830000	12.2516130000
1.4752570000	1.1649210000	12.3074350000
1.4550570000	3.9523450000	14.8683170000
3.9428830000	6.4633040000	3.9309720000
3.8572190000	9.6421370000	1.2114900000
1.2277220000	6.5567170000	1.4063410000
1.2502590000	9.5332270000	3.9509630000
4.0151190000	6.4633040000	9.3669640000
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1.2999580000	6.5567170000	6.8423330000
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4.0016910000	9.6421370000	12.0834760000
1.3721950000	6.5567170000	12.2783260000
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4.1388070000	12.0896320000	3.9851010000
4.2318680000	14.8107160000	1.4353590000
1.2707630000	12.1303950000	1.4095370000
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4.2110440000	12.0896320000	9.4210940000
4.3041040000	14.8107160000	6.8713520000
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4.3763400000	14.8107160000	12.3073440000
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9.7029320000	1.1693250000	4.1589020000
9.7195820000	3.9082810000	1.6215990000
6.8012390000	1.1693250000	1.4958670000
6.7845910000	3.9082810000	4.0331700000
9.7751680000	1.1693250000	9.5948930000
9.7918180000	3.9082810000	7.0575920000
6.8734750000	1.1693250000	6.9318590000
6.8568270000	3.9082810000	9.4691630000
9.8474040000	1.1693250000	15.0308870000
9.8640540000	3.9082810000	12.4935840000
6.9457110000	1.1693250000	12.3678520000
6.9290630000	3.9082810000	14.9051550000
10.0298190000	6.7727580000	4.8043910000
9.9855120000	9.6494370000	1.8942690000
6.4743530000	6.7727580000	0.8503780000
6.5186610000	9.6494370000	3.7604990000
10.1020560000	6.7727580000	10.2403840000
10.0577480000	9.6494370000	7.3302620000
6.5465890000	6.7727580000	6.2863710000
6.5908980000	9.6494370000	9.1964910000
10.1742920000	6.7727580000	15.6763760000
10.1299840000	9.6494370000	12.7662540000
6.6188250000	6.7727580000	11.7223630000
6.6631340000	9.6494370000	14.6324830000
9.7107930000	11.9830710000	4.2352510000
9.6745920000	14.7719360000	1.6059280000
6.7933800000	11.9830710000	1.4195170000
6.8295800000	14.7719360000	4.0488410000
9.7830290000	11.9830710000	9.6712440000
9.7468280000	14.7719360000	7.0419210000
6.8656160000	11.9830710000	6.8555100000
6.9018160000	14.7719360000	9.4848330000
9.8552650000	11.9830710000	15.1072360000

9.8190640000	14.7719360000	12.4779130000
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6.9740520000	14.7719360000	14.9208250000
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12.3832300000	3.9760830000	4.2751420000
15.2456240000	1.1649210000	9.6553110000
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12.3177460000	1.1969040000	7.0686260000
12.4554660000	3.9760830000	9.7111340000
15.3178600000	1.1649210000	15.0913040000
15.3380600000	3.9523450000	12.5304230000
12.3899820000	1.1969040000	12.5046200000
12.5277020000	3.9760830000	15.1471260000
15.2764490000	6.5567170000	4.2484270000
15.2539130000	9.5332270000	1.7038050000
12.5612900000	6.4633040000	1.7237970000
12.6469530000	9.6421370000	4.4432780000
15.3486850000	6.5567170000	9.6844200000
15.3261490000	9.5332270000	7.1397980000
12.6335260000	6.4633040000	7.1597900000
12.7191890000	9.6421370000	9.8792710000
15.4209220000	6.5567170000	15.1204130000
15.3983850000	9.5332270000	12.5757900000
12.7057620000	6.4633040000	12.5957820000
12.7914250000	9.6421370000	15.3152640000
15.2334090000	12.1303950000	4.2452310000
15.1362300000	14.8907270000	1.6618720000
12.3653650000	12.0896320000	1.6696670000
12.2723040000	14.8107160000	4.2194090000
15.3056450000	12.1303950000	9.6812240000
15.2084670000	14.8907270000	7.0978640000
12.4376010000	12.0896320000	7.1056600000
12.3445400000	14.8107160000	9.6554010000
15.3778810000	12.1303950000	15.1172160000
15.2807030000	14.8907270000	12.5338570000
12.5098370000	12.0896320000	12.5416530000
12.4167770000	14.8107160000	15.0913940000

Bulk CTS: Model-3 Structural parameters (VASP)

Cu Sn S

```
1.0000000000000000
16.4148186127710858 -0.0000000000000000 -0.0000000000000000
0.0000000000000000 16.4148186127710858 -0.0000000000000000
0.0000000000000000 -0.0000000000000000 16.3814274087187606
```

72 36 108

Cartesian

```
0.0000000000 0.0000000000 0.0000000000
0.0000000000 2.7358030000 2.3552690000
2.7358030000 0.0000000000 2.3552690000
0.0000000000 2.7358030000 8.1907140000
2.7358030000 0.0000000000 8.1907140000
0.0000000000 2.7358030000 14.0261590000
2.7358030000 0.0000000000 14.0261590000
0.0000000000 5.4716060000 0.0000000000
0.0000000000 8.2074090000 2.3552690000
2.7358030000 5.4716060000 2.3552690000
0.0000000000 8.2074090000 8.1907140000
2.7358030000 5.4716060000 8.1907140000
0.0000000000 8.2074090000 14.0261590000
2.7358030000 5.4716060000 14.0261590000
0.0000000000 10.9432130000 0.0000000000
0.0000000000 13.6790140000 2.3552690000
2.7358030000 10.9432130000 2.3552690000
0.0000000000 13.6790140000 8.1907140000
2.7358030000 10.9432130000 8.1907140000
0.0000000000 13.6790140000 14.0261590000
2.7358030000 10.9432130000 14.0261590000
5.4716060000 0.0000000000 0.0000000000
5.4716060000 2.7358030000 2.3552690000
8.2074090000 0.0000000000 2.3552690000
5.4716060000 2.7358030000 8.1907140000
8.2074090000 0.0000000000 8.1907140000
5.4716060000 2.7358030000 14.0261590000
8.2074090000 0.0000000000 14.0261590000
5.4716060000 5.4716060000 0.0000000000
5.4716060000 10.9432130000 0.0000000000
5.4716060000 13.6790140000 2.3552690000
8.2074090000 10.9432130000 2.3552690000
5.4716060000 13.6790140000 8.1907140000
8.2074090000 10.9432130000 8.1907140000
5.4716060000 13.6790140000 14.0261590000
8.2074090000 10.9432130000 14.0261590000
10.9432130000 0.0000000000 0.0000000000
10.9432130000 2.7358030000 2.3552690000
13.6790140000 0.0000000000 2.3552690000
10.9432130000 2.7358030000 8.1907140000
13.6790140000 0.0000000000 8.1907140000
10.9432130000 2.7358030000 14.0261590000
13.6790140000 0.0000000000 14.0261590000
10.9432130000 5.4716060000 0.0000000000
13.6790140000 5.4716060000 2.3552690000
13.6790140000 5.4716060000 8.1907140000
13.6790140000 5.4716060000 14.0261590000
10.9432130000 10.9432130000 0.0000000000
10.9432130000 13.6790140000 2.3552690000
13.6790140000 10.9432130000 2.3552690000
10.9432130000 13.6790140000 8.1907140000
13.6790140000 10.9432130000 8.1907140000
10.9432130000 13.6790140000 14.0261590000
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13.6790140000	10.9432130000	14.0261590000
5.4716060000	8.2074090000	2.3552690000
8.2074090000	5.4716060000	2.3552690000
5.4716060000	8.2074090000	8.1907140000
8.2074090000	5.4716060000	8.1907140000
5.4716060000	8.2074090000	14.0261590000
8.2074090000	5.4716060000	14.0261590000
10.9432130000	8.2074090000	2.3552690000
10.9432130000	8.2074090000	8.1907140000
10.9432130000	8.2074090000	14.0261590000
2.7358030000	2.7358030000	0.0000000000
2.7358030000	8.2074090000	0.0000000000
2.7358030000	13.6790140000	0.0000000000
8.2074090000	2.7358030000	0.0000000000
8.2074090000	8.2074090000	0.0000000000
8.2074090000	13.6790140000	0.0000000000
13.6790140000	2.7358030000	0.0000000000
13.6790140000	8.2074090000	0.0000000000
13.6790140000	13.6790140000	0.0000000000
0.0000000000	0.0000000000	5.2671290000
0.0000000000	5.4716060000	5.2671290000
0.0000000000	10.9432130000	5.2671290000
5.4716060000	0.0000000000	5.2671290000
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5.4716060000	10.9432130000	5.2671290000
10.9432130000	0.0000000000	5.2671290000
10.9432130000	5.4716060000	5.2671290000
10.9432130000	10.9432130000	5.2671290000
2.7358030000	2.7358030000	5.2671290000
2.7358030000	8.2074090000	5.2671290000
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8.2074090000	8.2074090000	5.2671290000
8.2074090000	13.6790140000	5.2671290000
13.6790140000	2.7358030000	5.2671290000
13.6790140000	8.2074090000	5.2671290000
13.6790140000	13.6790140000	5.2671290000
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0.0000000000	5.4716060000	11.1142990000
0.0000000000	10.9432130000	11.1142990000
5.4716060000	0.0000000000	11.1142990000
5.4716060000	5.4716060000	11.1142990000
5.4716060000	10.9432130000	11.1142990000
10.9432130000	0.0000000000	11.1142990000
10.9432130000	5.4716060000	11.1142990000
10.9432130000	10.9432130000	11.1142990000
2.7358030000	2.7358030000	11.1142990000
2.7358030000	8.2074090000	11.1142990000
2.7358030000	13.6790140000	11.1142990000
8.2074090000	2.7358030000	11.1142990000
8.2074090000	8.2074090000	11.1142990000
8.2074090000	13.6790140000	11.1142990000
13.6790140000	2.7358030000	11.1142990000
13.6790140000	8.2074090000	11.1142990000
13.6790140000	13.6790140000	11.1142990000
4.1037040000	1.3679020000	3.6009640000
4.1037040000	4.1037040000	1.2063430000
1.3679020000	1.3679020000	1.2063430000
1.3679020000	4.1037040000	3.6009640000
4.1037040000	1.3679020000	9.3997130000
4.1037040000	4.1037040000	6.9817160000
1.3679020000	1.3679020000	6.9817160000

1.3679020000	4.1037040000	9.3997130000
4.1037040000	1.3679020000	15.1750850000
4.1037040000	4.1037040000	12.7804640000
1.3679020000	1.3679020000	12.7804640000
1.3679020000	4.1037040000	15.1750850000
4.1037040000	6.8395070000	3.6009640000
4.1037040000	9.5753100000	1.2063430000
1.3679020000	6.8395070000	1.2063430000
1.3679020000	9.5753100000	3.6009640000
4.1037040000	6.8395070000	9.3997130000
4.1037040000	9.5753100000	6.9817160000
1.3679020000	6.8395070000	6.9817160000
1.3679020000	9.5753100000	9.3997130000
4.1037040000	6.8395070000	15.1750850000
4.1037040000	9.5753100000	12.7804640000
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1.3679020000	12.3111130000	12.7804640000
1.3679020000	15.0469170000	15.1750850000
9.5753100000	1.3679020000	3.6009640000
9.5753100000	4.1037040000	1.2063430000
6.8395070000	1.3679020000	1.2063430000
6.8395070000	4.1037040000	3.6009640000
9.5753100000	1.3679020000	9.3997130000
9.5753100000	4.1037040000	6.9817160000
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6.8395070000	4.1037040000	9.3997130000
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9.5753100000	4.1037040000	12.7804640000
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9.5753100000	9.5753100000	1.2063430000
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6.8395070000	9.5753100000	15.1750850000
9.5753100000	12.3111130000	3.6009640000
9.5753100000	15.0469170000	1.2063430000
6.8395070000	12.3111130000	1.2063430000
6.8395070000	15.0469170000	3.6009640000
9.5753100000	12.3111130000	9.3997130000
9.5753100000	15.0469170000	6.9817160000
6.8395070000	12.3111130000	6.9817160000
6.8395070000	15.0469170000	9.3997130000
9.5753100000	12.3111130000	15.1750850000

9.575310000	15.046917000	12.780464000
6.839507000	12.311113000	12.780464000
6.839507000	15.046917000	15.175085000
15.046917000	1.367902000	3.600964000
15.046917000	4.103704000	1.206343000
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15.046917000	4.103704000	6.981716000
12.311113000	1.367902000	6.981716000
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12.311113000	9.575310000	9.399713000
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15.046917000	9.575310000	12.780464000
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12.311113000	9.575310000	15.175085000
15.046917000	12.311113000	3.600964000
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15.046917000	12.311113000	9.399713000
15.046917000	15.046917000	6.981716000
12.311113000	12.311113000	6.981716000
12.311113000	15.046917000	9.399713000
15.046917000	12.311113000	15.175085000
15.046917000	15.046917000	12.780464000
12.311113000	12.311113000	12.780464000
12.311113000	15.046917000	15.175085000

Bulk CdS: Structural parameters (VASP)

Cd S

```
1.0000000000000000
 4.1560896338577944  0.000000069236663 -0.0000000000000000
-2.0780453049367553  3.5992790341404586  0.0000000000000000
 0.0000000000000000  0.0000000000000000  6.7600040349108603
 2 2
```

Cartesian

```
-0.0000030000  2.3995200000  0.0012320000
2.0780470000  1.1997580000  3.3812340000
-0.0000030000  2.3995200000  2.5472890000
2.0780470000  1.1997580000  5.9272910000
```

Bulk ZnS: Structural parameters (VASP)

Zn S

```
1.0000000000000000
 5.4074360910337922 -0.0000000000000000 -0.0000000000000000
 0.0000000000000000  5.4074360910337922  0.0000000000000000
-0.0000000000000000  0.0000000000000000  5.4074360910337922
 4 4
```

Cartesian

```
0.0000000000  0.0000000000  0.0000000000
0.0000000000  2.6937180000  2.6937180000
2.6937180000  0.0000000000  2.6937180000
2.6937180000  2.6937180000  0.0000000000
4.0405770000  1.3468590000  4.0405770000
4.0405770000  4.0405770000  1.3468590000
1.3468590000  1.3468590000  1.3468590000
1.3468590000  4.0405770000  4.0405770000
```

CTS (111) surface: Structural parameters (VASP)

Cu Sn S

1.0

22.8522052765	0.0000000000	0.0000000000
11.3051514310	19.8729397395	0.0000000000
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44 71 216

Cartesian

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14.865843829	-1.090527651	12.898182198
7.320686867	-1.060479873	12.903403272
18.693674919	5.338437761	12.903598366
26.586376190	-1.079796100	12.912794471
13.112221099	-4.495157134	12.936914069
28.386976655	2.011225478	12.949422119
18.727220732	-7.650203116	12.979036851
22.692837409	5.341273075	12.980477989
20.672080770	1.936071717	12.981218880
24.571617852	-4.456542622	12.989479000
11.137274901	5.540048424	12.992830428

20.734930323	-4.365286826	13.068930838
26.296150811	5.408483959	13.071930401
5.533123447	-4.318780728	13.073996302
22.654472931	-7.451580788	13.088023294
30.295324421	5.481002743	13.097609586
16.833634427	2.120646293	13.098271511
9.315871559	2.176251124	13.109103846
24.548518574	2.067863788	13.160500539
28.261227179	8.749743336	13.258732451
32.045008484	8.728767251	13.408438861
13.062810638	8.863405193	13.585344559
3.771764529	-7.453251588	13.592124059
11.059860000	-5.965362339	15.616825561
15.029367141	-5.483764618	15.765830563
9.305584882	-9.343948091	15.851828486
13.066914103	-2.211785709	15.941176675
20.717290949	-2.220844943	15.987078233
18.956631036	-5.439100022	15.987935251
13.175588238	-9.215351519	16.033174884
18.767884587	7.778920482	16.039525875
15.047703695	1.247046617	16.043540389
26.318246697	1.264559125	16.043773805
22.670727851	1.267396007	16.047592064
16.820915597	4.340396365	16.054060343
16.959362920	-9.066212774	16.057879763
18.634235943	1.232345674	16.059165290
11.089067189	1.262372723	16.064386365
22.462055923	7.661290358	16.064581458
7.502550384	1.243082648	16.073738080
16.880600740	-2.172304537	16.097897161
9.303150934	4.334104226	16.110365728
22.495601055	-5.327349751	16.140018782
26.461229187	7.664145808	16.141461081
24.440461092	4.258950465	16.142162488
5.487803844	-2.133670185	16.150462092
14.905666338	7.862921157	16.153813520
24.503310814	-2.042407782	16.229874447
30.064552927	7.731336555	16.232913493
9.301503597	-1.995901684	16.234939911
3.570648229	-5.128701596	16.248966903
11.211498700	7.803856108	16.258591517
20.602016104	4.443500074	16.259254603
13.084251881	4.499103720	16.270086938
28.316898896	4.390717153	16.321482469
20.724467441	-8.800323818	16.419715543
1.656031846	-8.821294954	16.569383631
5.526039021	-8.686656095	16.746288168
7.540156050	-5.130378707	16.753107151

CdS (100) surface: Structural parameters (VASP)

Cd S

1.0

8.3121795654	0.0000000000	0.0000000000
0.0000000000	13.5200080872	0.0000000000
12.4682638491	0.0000000000	36.5956770618

48 48

Cartesian

0.000000000	0.001230321	0.000000000
2.078036350	3.381232160	1.199752678
2.078048500	0.001230321	3.599294571
4.156084912	3.381232160	4.799047249
4.156084552	0.001230321	7.198552606
6.234120902	3.381232160	8.398305284
6.234133299	0.001230321	10.797847722
4.156079635	3.381232160	11.997599855
8.312177278	0.001230321	14.397105211
6.234136418	3.381232160	15.596894426
6.234136073	0.001230321	17.996399782
8.312172346	3.381232160	19.196151915
0.000000000	6.761234585	0.000000000
2.078036350	10.141236606	1.199752678
2.078048500	6.761234585	3.599294571
4.156084912	10.141236606	4.799047249
4.156084552	6.761234585	7.198552606
6.234120902	10.141236606	8.398305284
6.234133299	6.761234585	10.797847722
4.156079635	10.141236606	11.997599855
8.312177278	6.761234585	14.397105211
6.234136418	10.141236606	15.596894426
6.234136073	6.761234585	17.996399782
8.312172346	10.141236606	19.196151915
4.156089783	0.001230321	0.000000000
6.234126257	3.381232160	1.199752678
6.234138221	0.001230321	3.599294571
8.312174695	3.381232160	4.799047249
8.312174211	0.001230321	7.198552606
10.390210685	3.381232160	8.398305284
10.390231257	0.001230321	10.797847722
8.312177763	3.381232160	11.997599855
12.468267061	0.001230321	14.397105211
10.390226201	3.381232160	15.596894426
10.390225716	0.001230321	17.996399782
12.468262005	3.381232160	19.196151915
4.156089783	6.761234585	0.000000000
6.234126257	10.141236606	1.199752678
6.234138221	6.761234585	3.599294571
8.312174695	10.141236606	4.799047249
8.312174211	6.761234585	7.198552606
10.390210685	10.141236606	8.398305284
10.390231257	6.761234585	10.797847722
8.312177763	10.141236606	11.997599855
12.468267061	6.761234585	14.397105211
10.390226201	10.141236606	15.596894426

10.390225716	6.761234585	17.996399782
12.468262005	10.141236606	19.196151915
0.000000000	2.547291212	0.000000000
2.078036350	5.927293234	1.199752678
2.078048500	2.547291212	3.599294571
4.156084912	5.927293234	4.799047249
4.156084552	2.547291212	7.198552606
6.234120902	5.927293234	8.398305284
6.234133299	2.547291212	10.797847722
4.156079635	5.927293234	11.997599855
8.312177278	2.547291212	14.397105211
6.234136418	5.927293234	15.596894426
6.234136073	2.547291212	17.996399782
8.312172346	5.927293234	19.196151915
0.000000000	9.307294853	0.000000000
2.078036350	12.687296875	1.199752678
2.078048500	9.307294853	3.599294571
4.156084912	12.687296875	4.799047249
4.156084552	9.307294853	7.198552606
6.234120902	12.687296875	8.398305284
6.234133299	9.307294853	10.797847722
4.156079635	12.687296875	11.997599855
8.312177278	9.307294853	14.397105211
6.234136418	12.687296875	15.596894426
6.234136073	9.307294853	17.996399782
8.312172346	12.687296875	19.196151915
4.156089783	2.547291212	0.000000000
6.234126257	5.927293234	1.199752678
6.234138221	2.547291212	3.599294571
8.312174695	5.927293234	4.799047249
8.312174211	2.547291212	7.198552606
10.390210685	5.927293234	8.398305284
10.390231257	2.547291212	10.797847722
8.312177763	5.927293234	11.997599855
12.468267061	2.547291212	14.397105211
10.390226201	5.927293234	15.596894426
10.390225716	2.547291212	17.996399782
12.468262005	5.927293234	19.196151915
4.156089783	9.307294853	0.000000000
6.234126257	12.687296875	1.199752678
6.234138221	9.307294853	3.599294571
8.312174695	12.687296875	4.799047249
8.312174211	9.307294853	7.198552606
10.390210685	12.687296875	8.398305284
10.390231257	9.307294853	10.797847722
8.312177763	12.687296875	11.997599855
12.468267061	9.307294853	14.397105211
10.390226201	12.687296875	15.596894426
10.390225716	9.307294853	17.996399782
12.468262005	12.687296875	19.196151915

ZnS (110) surface: Structural parameters (VASP)

Zn S

1.0

10.7748718262	0.0000000000	0.0000000000
0.0000000000	15.2379703522	0.0000000000
0.0000000000	22.8569548267	42.8569553302

96 96

Cartesian

2.686337101	5.696303874	0.009771386
5.378923765	7.625232767	1.915277409
5.390593128	11.423921875	1.900105911
2.691627651	5.713728381	3.811911950
2.696777873	9.524089317	3.807111775
5.387985664	11.428104492	5.713817808
5.386153696	15.238396570	5.714889409
2.694181327	9.523975325	7.618681107
2.693491730	13.333078953	7.619152407
5.387274392	15.238091902	9.523843918
5.387511054	19.047485831	9.523629981
2.693750389	13.333277458	11.428536067
2.693750389	17.142777539	11.428407066
5.387274392	19.047592829	13.333099215
5.387511054	7.619007834	13.333355940
2.693491730	17.142564264	15.237790088
2.694181327	20.952429918	15.238261388
5.387985664	22.856588994	17.143124687
5.386153696	11.428904136	17.142096511
2.696777873	20.952574495	19.049831039
2.691627651	24.761198338	19.045031183
5.378923765	11.434717239	20.941665245
5.390593128	15.233413981	20.956879690
2.686337101	24.743773426	22.847170994
2.686337101	13.315288596	0.009771386
5.378923765	15.244217943	1.915277409
5.390593128	3.804936472	1.900105911
2.691627651	13.332713784	3.811911950
2.696777873	17.143074947	3.807111775
5.387985664	3.809119145	5.713817808
5.386153696	7.619411848	5.714889409
2.694181327	17.142960501	7.618681107
2.693491730	5.714094004	7.619152407
5.387274392	7.619106953	9.523843918
5.387511054	11.428500655	9.523629981
2.693750389	20.952262634	11.428536067
2.693750389	9.523792136	11.428407066
5.387274392	11.428607199	13.333099215
5.387511054	15.237992840	13.333355940
2.693491730	9.523578634	15.237790088
2.694181327	13.333444287	15.238261388
5.387985664	15.237604272	17.143124687
5.386153696	19.047889539	17.142096511
2.696777873	13.333589546	19.049831039
2.691627651	17.142213616	19.045031183
5.378923765	19.053702528	20.941665245
5.390593128	22.852398703	20.956879690

2.686337101	17.124773264	22.847170994
8.073773335	5.696303874	0.009771386
10.766359678	7.625232767	1.915277409
0.003157037	11.423921875	1.900105911
8.079063403	5.713728381	3.811911950
8.084214107	9.524089317	3.807111775
0.000549518	11.428104492	5.713817808
10.773589930	15.238396570	5.714889409
8.081616919	9.523975325	7.618681107
8.080927804	13.333078953	7.619152407
10.774709984	15.238091902	9.523843918
0.000075424	19.047485831	9.523629981
8.081185981	13.333277458	11.428536067
8.081185981	17.142777539	11.428407066
10.774709984	19.047592829	13.333099215
0.000075424	7.619007834	13.33355940
8.080927804	17.142564264	15.237790088
8.081616919	20.952429918	15.238261388
0.000549518	22.856588994	17.143124687
10.773589930	11.428904136	17.142096511
8.084214107	20.952574495	19.049831039
8.079063403	24.761198338	19.045031183
10.766359678	11.434717239	20.941665245
0.003157037	15.233413981	20.956879690
8.073773335	24.743773426	22.847170994
8.073773335	13.315288596	0.009771386
10.766359678	15.244217943	1.915277409
0.003157037	3.804936472	1.900105911
8.079063403	13.332713784	3.811911950
8.084214107	17.143074947	3.807111775
0.000549518	3.809119145	5.713817808
10.773589930	7.619411848	5.714889409
8.081616919	17.142960501	7.618681107
8.080927804	5.714094004	7.619152407
10.774709984	7.619106953	9.523843918
0.000075424	11.428500655	9.523629981
8.081185981	20.952262634	11.428536067
8.081185981	9.523792136	11.428407066
10.774709984	11.428607199	13.333099215
0.000075424	15.237992840	13.33355940
8.080927804	9.523578634	15.237790088
8.081616919	13.333444287	15.238261388
0.000549518	15.237604272	17.143124687
10.773589930	19.047889539	17.142096511
8.084214107	13.333589546	19.049831039
8.079063403	17.142213616	19.045031183
10.766359678	19.053702528	20.941665245
0.003157037	22.852398703	20.956879690
8.073773335	17.124773264	22.847170994
1.350824121	26.679079409	42.852668923
4.042882870	5.721057992	1.898434487
4.043378353	9.520272156	1.899420195
1.347570090	11.430161491	3.811569012
1.349110966	7.617407761	3.806254749
4.040458443	9.523556311	5.715789223
4.040910896	13.333376097	5.713603870

1.346934441	15.237886328	7.618466531
1.346848221	11.428576639	7.619409770
4.040587853	13.333269542	9.523587193
4.040555420	17.142663585	9.523972919
1.346858978	19.047454806	11.428621642
1.346858978	15.237954725	11.428321491
4.040587853	17.142739134	13.333355940
4.040555420	20.952147709	13.332970215
1.346848221	22.857054506	15.237576789
1.346934441	19.047363464	15.238519390
4.040458443	20.952041381	17.141153911
4.040910896	9.523891184	17.143339263
1.349110966	11.426900610	19.050731491
1.347570090	22.858646385	19.045373482
4.042882870	24.768520649	20.958551593
4.043378353	13.329772124	20.957522140
1.350824121	15.250602426	22.861271689
1.350824121	34.298064585	42.852668923
4.042882870	13.340042714	1.898434487
4.043378353	1.901287207	1.899420195
1.347570090	3.811176315	3.811569012
1.349110966	15.236392937	3.806254749
4.040458443	17.142541033	5.715789223
4.040910896	5.714391375	5.713603870
1.346934441	7.618901151	7.618466531
1.346848221	19.047562269	7.619409770
4.040587853	5.714284593	9.523587193
4.040555420	9.523677954	9.523972919
1.346858978	11.428470084	11.428621642
1.346858978	7.618969776	11.428321491
4.040587853	9.523754185	13.333355940
4.040555420	13.333162987	13.332970215
1.346848221	15.238069329	15.237576789
1.346934441	11.428378742	15.238519390
4.040458443	13.333056205	17.141153911
4.040910896	17.142875991	17.143339263
1.349110966	19.045870686	19.050731491
1.347570090	15.239661209	19.045373482
4.042882870	17.149535473	20.958551593
4.043378353	20.948757073	20.957522140
1.350824121	22.869587148	22.861271689
6.738260034	26.679079409	42.852668923
9.430318462	5.721057992	1.898434487
9.430814266	9.520272156	1.899420195
6.735005843	11.430161491	3.811569012
6.736546558	7.617407761	3.806254749
9.427894035	9.523556311	5.715789223
9.428346809	13.333376097	5.713603870
6.734370033	15.237886328	7.618466531
6.734283973	11.428576639	7.619409770
9.428023766	13.333269542	9.523587193
9.427991012	17.142663585	9.523972919
6.734294891	19.047454806	11.428621642
6.734294891	15.237954725	11.428321491
9.428023766	17.142739134	13.333355940
9.427991012	20.952147709	13.332970215

6.734283973	22.857054506	15.237576789
6.734370033	19.047363464	15.238519390
9.427894035	20.952041381	17.141153911
9.428346809	9.523891184	17.143339263
6.736546558	11.426900610	19.050731491
6.735005843	22.858646385	19.045373482
9.430318462	24.768520649	20.958551593
9.430814266	13.329772124	20.957522140
6.738260034	15.250602426	22.861271689
6.738260034	34.298064585	42.852668923
9.430318462	13.340042714	1.898434487
9.430814266	1.901287207	1.899420195
6.735005843	3.811176315	3.811569012
6.736546558	15.236392937	3.806254749
9.427894035	17.142541033	5.715789223
9.428346809	5.714391375	5.713603870
6.734370033	7.618901151	7.618466531
6.734283973	19.047562269	7.619409770
9.428023766	5.714284593	9.523587193
9.427991012	9.523677954	9.523972919
6.734294891	11.428470084	11.428621642
6.734294891	7.618969776	11.428321491
9.428023766	9.523754185	13.333355940
9.427991012	13.333162987	13.332970215
6.734283973	15.238069329	15.237576789
6.734370033	11.428378742	15.238519390
9.427894035	13.333056205	17.141153911
9.428346809	17.142875991	17.143339263
6.736546558	19.045870686	19.050731491
6.735005843	15.239661209	19.045373482
9.430318462	17.149535473	20.958551593
9.430814266	20.948757073	20.957522140
6.738260034	22.869587148	22.861271689