Fabrication of novel $CuAgZnSnSe_4$-$Cu_2ZnSnSe_4$ thin film solar cells by vacuum evaporation method.

Johnson Henry[a], Kannusamy Mohanraj[a,*] and Ganesan Sivakumar[b]

[a]Department of Physics, Manonmaniam Sundaranar University, Tirunelveli 627 012, Tamil Nadu, India

[b]Centralised Instrumentation and Service Laboratory (CISL), Department of Physics, Annamalai University, Annamalai Nagar 608 002, Tamil Nadu, India

* Corresponding author: mohanraj@msuniv.ac.in; kmohanraj.msu@gmail.com

KEYWORDS: CAZTSe, Solar cell, Mott-Schottky plot, Bandgap engineering, Photoconversion efficiency, Thin film

Supporting Information

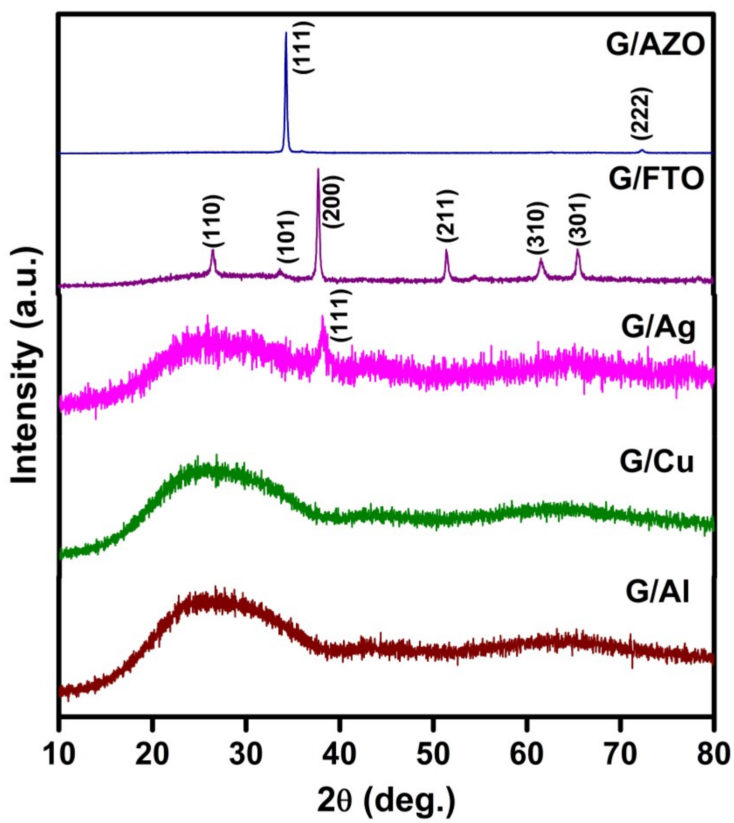

Fig. S1. XRD pattern of various conducting substrates

The substrates Al, Cu, Ag thin films were deposited by thermal evaporation method and FTO & AZO are commercial substrates purchased from chemical companies. Fig. S1 shows the XRD pattern of all substrates. The XRD pattern of Al & Cu shows amorphous nature, while the Ag substrate shows a polycrystalline peak at 2θ=38.1˚ belongs to the cubic Ag (JCPDS card No.: 040783). The XRD pattern of FTO substrates if given in Fig. 6 for comparison purpose and it is well matched with JCPDS card no. 461088. The XRD pattern shows prominent peaks at 2θ = 26.6˚, 33.8 ˚, 37.8 ˚, 51.5 ˚, 61.6 ˚ and 65.5˚ belongs to the diffraction of (110), (101), (200), (211), (310) and (310) planes respectively of tetragonal structured F doped SnO_2. The XRD pattern of the Al doped ZnO (AZO) substrates which shows prominat peak at 2θ = 34˚ belongs to the diffraction of (111) plane of cubic Al doped ZnO films. A small peak appears at 2θ = 72.4˚ belongs to the diffraction of (222) plane (JCPDS Card No.: 652880). The obtained peak position is sifted towards higher angle when compared with the JCPDS Card No.: 652880. The shift is due to the replacement of smaller ionic radii Al^{3+} (0.53 Å) into the lattice of bigger ionic radii Zn^{2+} (0.74 Å).

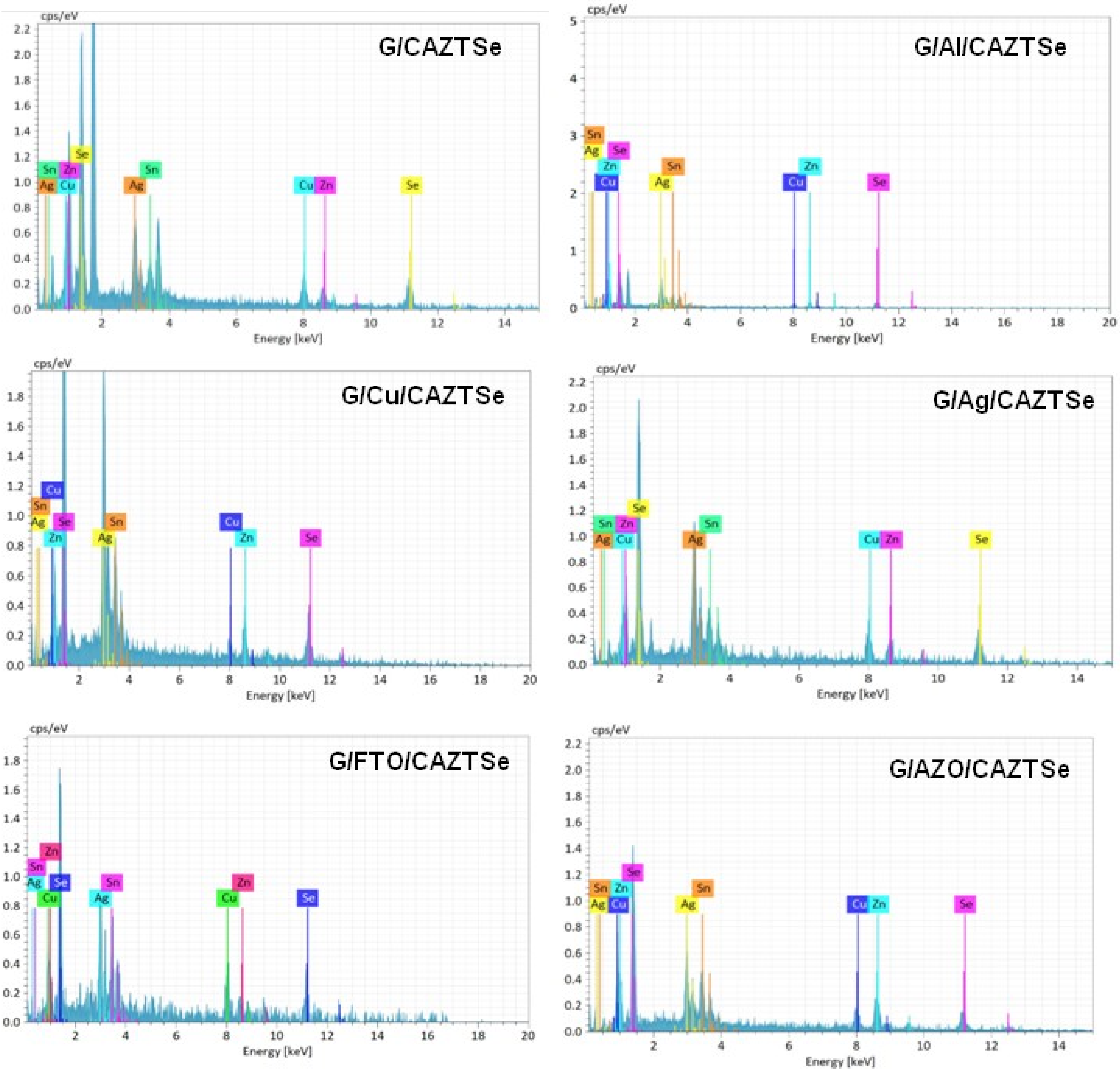

Fig. S2. EDS spectra of CAZTSe thin films deposited on various substrates

Table S1: EDS composition of CAZTSe thin films deposited on various substrates

Substrate	**Cu**	**Ag**	**Zn**	**Sn**	**Se**	**(Cu+Ag)/(Zn+Sn)**	**Zn/Sn**
Expectation	12.5	12.5	12.5	12.5	50	1	1
Glass	12.5	13	12	12	49	1.06	1
Al	11	25	12	13	39	1.44	0.92
Cu	20	28	11	11	30	2.18	1
Ag	13	22	14	11	40	1.4	1.27
FTO	22	10	12	10	46	1.45	1.2
AZO	16	20	19	17	28	1	1.11

Figure S3 shows the 3D AFM images of CAZTSe thin films depoited on various conducting substrates. From the figure the surface roughness values is found to be 27.3 mn, 30 nm, 62.5 nm, 41.2 nm, 23.3 nm and 27.6 nm for the CAZTSe thin films deposited on glass, Al, Cu, Ag, FTO and AZO substrates respectively. The film deposited on Cu substrate shows higher surface roughness, which introduce large nucleation sites and reduces the grain sizes and thus increases the grain boundaries. This leads to recombination in at the grain boundaries and increase in series resistances (Sun et al., 2014). The same information is given in supporting information.

Kaiwen Sun, Zhenghua Su, Chang Yan, Fangyang Liu, Hongtao Cui, Liangxing Jiang, Yansong Shen, Xiaojing Hao, Yexiang Liu, Flexible Cu2ZnSnS4 solar cells based on successive ionic layer adsorption and reaction method, RSC Adv., 2014, 4, 17703–17708

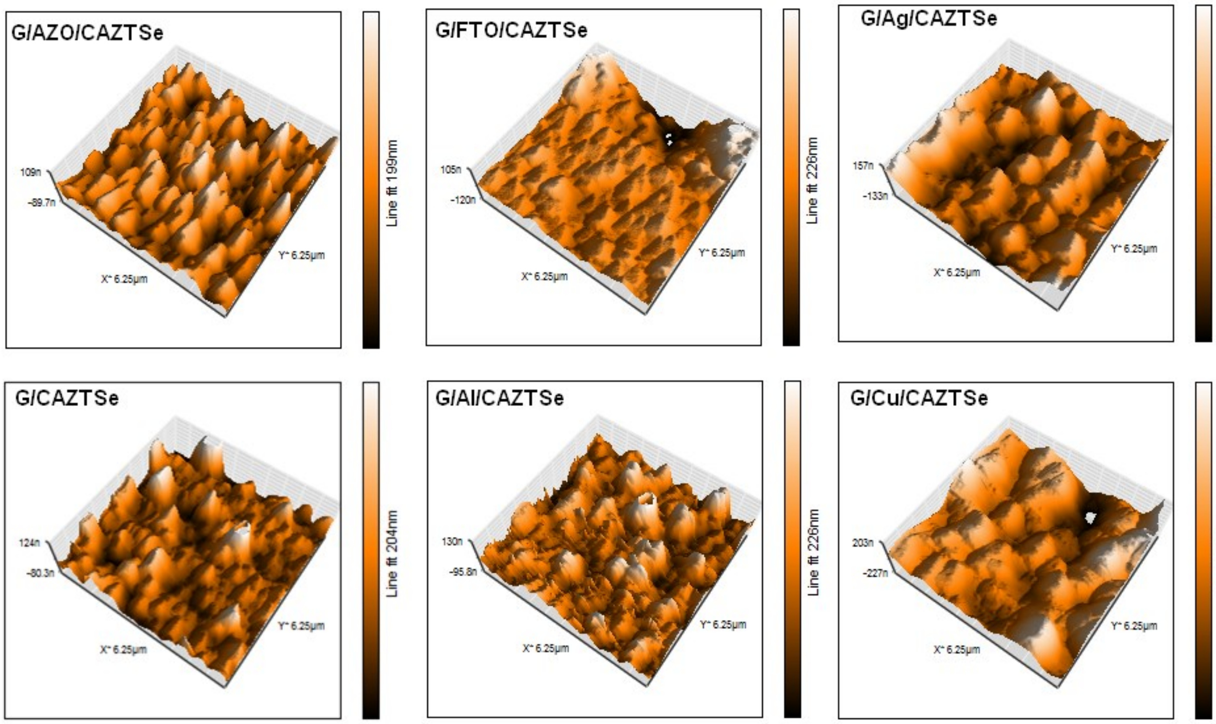

Figure S3: 3D AFM images of CAZTSe thin films deposited on various conducting substrates.

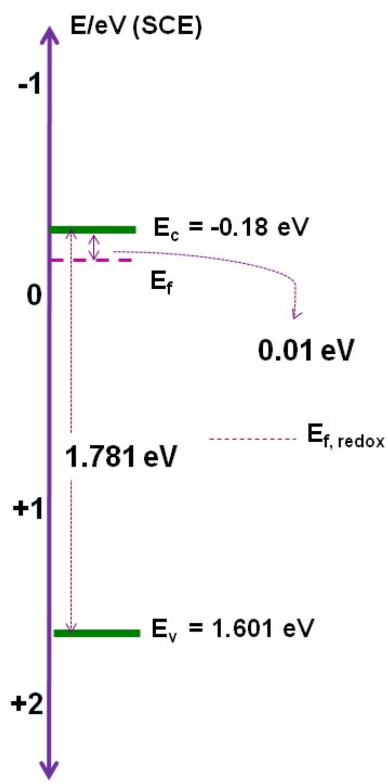

Fig. S4. Ag-CAZTSe/polysulphide band diagram at flat band condition

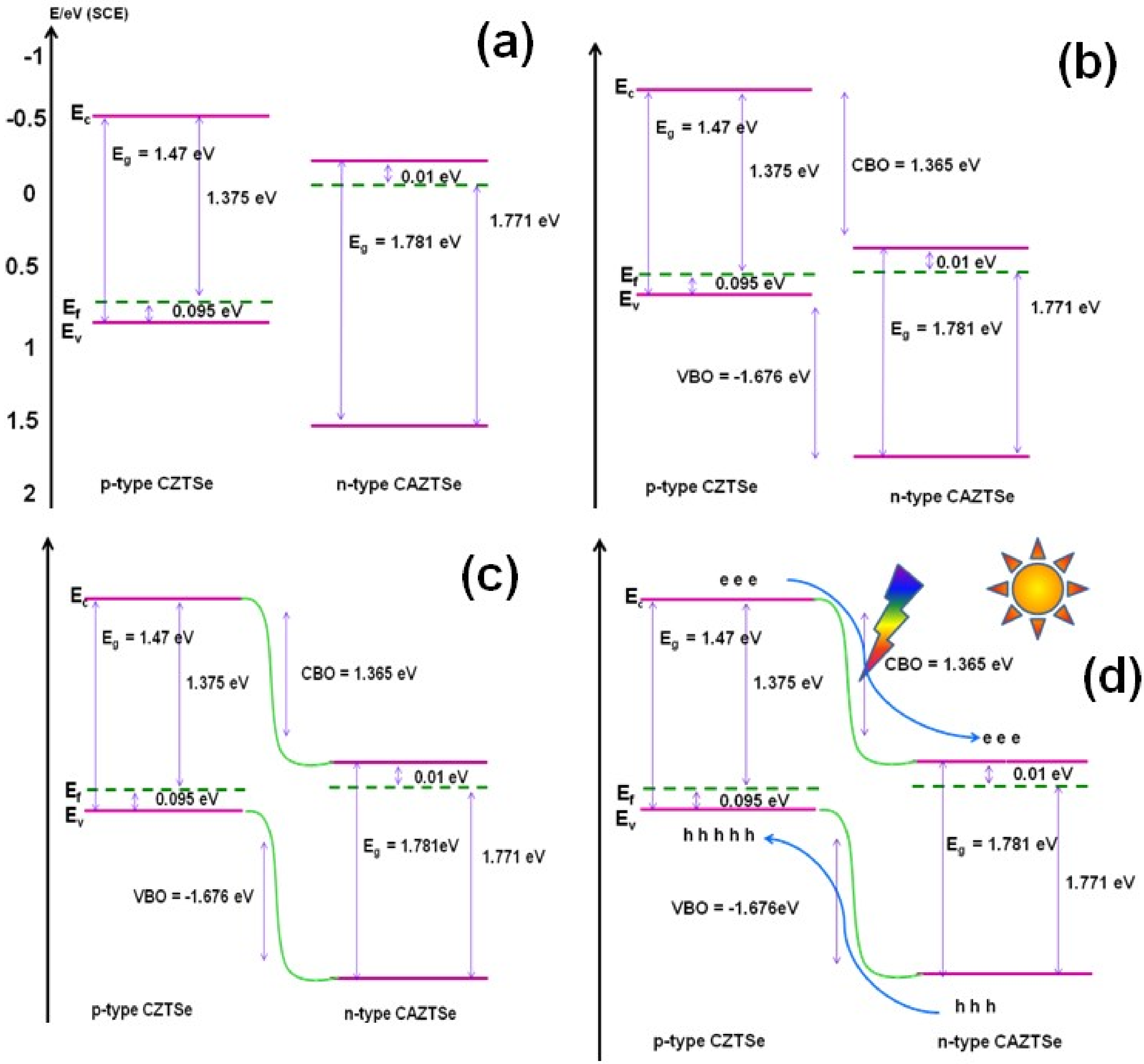

Fig. S5. (a) before and (b) after contact, (c) equilibrium position and (d) under the illumination of p-n junction solar cell for Ag/CAZTSe/CZTSe/Ag