Supplementary Materials: Hybrid density functional study of $Au_2Cs_2I_6$, Ag_2GeBaS_4, Ag_2ZnSnS_4 and $AgCuPO_4$ for the Intermediate band solar cells

Murugesan Rasukkannu [1,*], Dhayalan Velauthapillai [1], and Ponniah Vajeeston [2]

1. Supplementary data

From Figure S1, Ag_2GeBaS_4 IB is mainly contributed from the S-3p and small extraction from Ag-5s and Ba-6s states at 0.9 eV. The calculated DOS and PDOS values of Ag_2ZnSnS_4 presented in Figure S2, Ag-5s and Sn-5p states contribute the IB. From Fig.S3, we observed that the calculated DOS and PDOS of $AgCuPO_4$. The IB derived from Ag-4d and Cu-3d states.

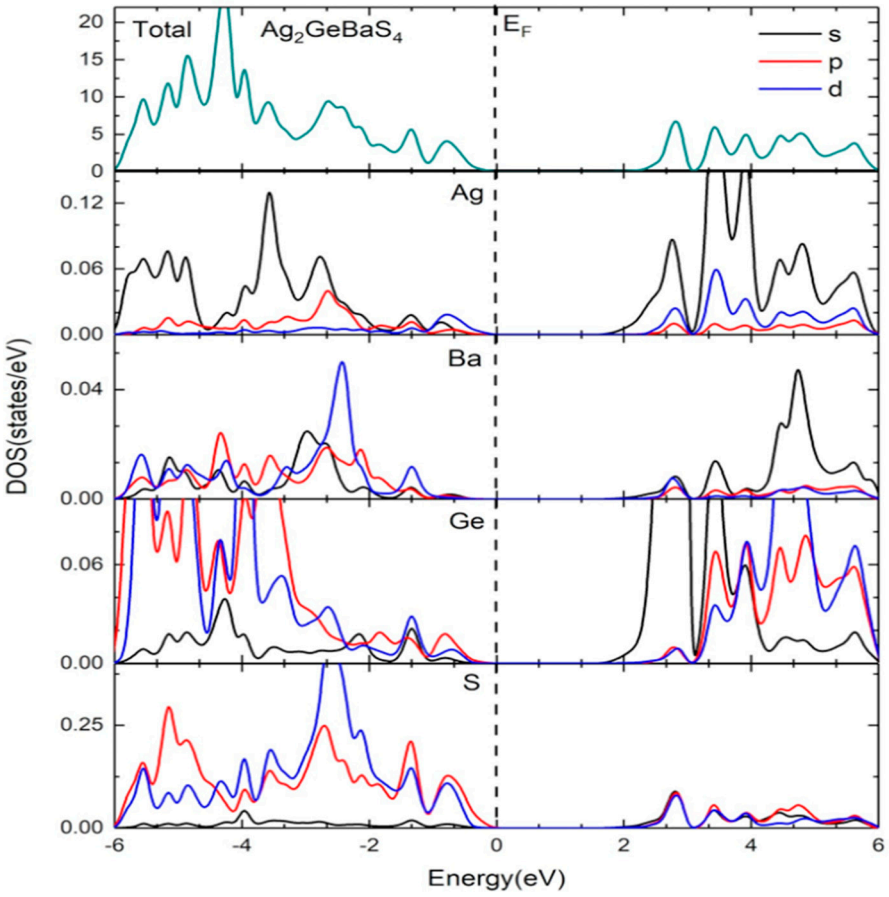

Figure S1. Calculated total and site projected density of states of Ag_2GeBaS_4. The Fermi level is set to zero and marked by a vertical dotted line.

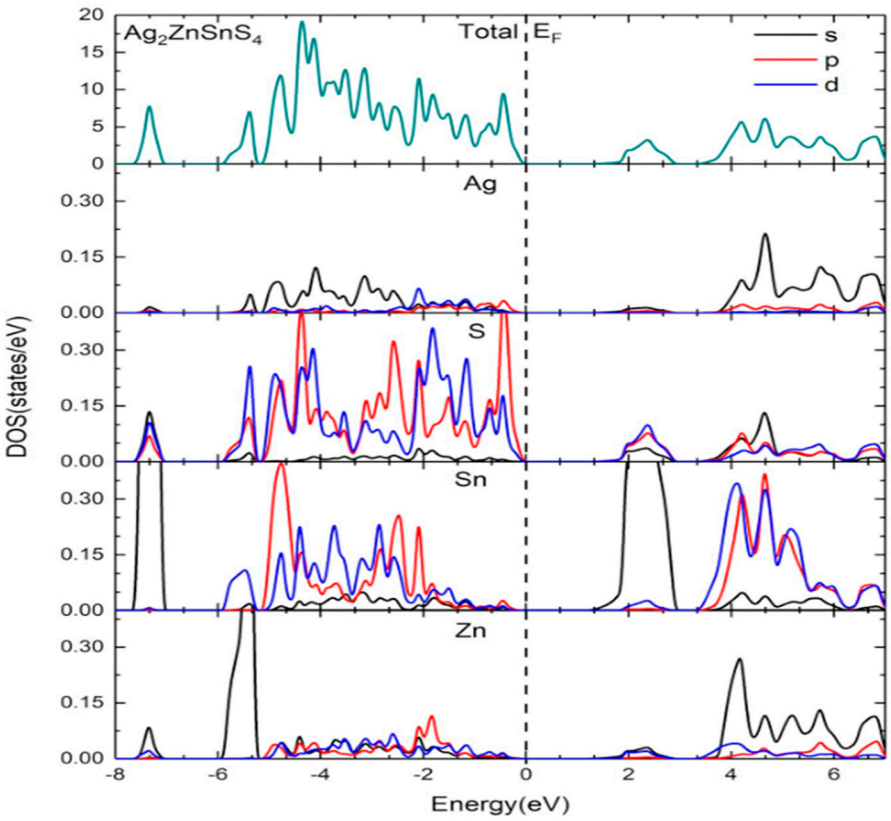

Figure S2. Calculated total and site projected density of states of Ag_2ZnSnS_4. The Fermi level is set to zero and marked by a vertical dotted line.

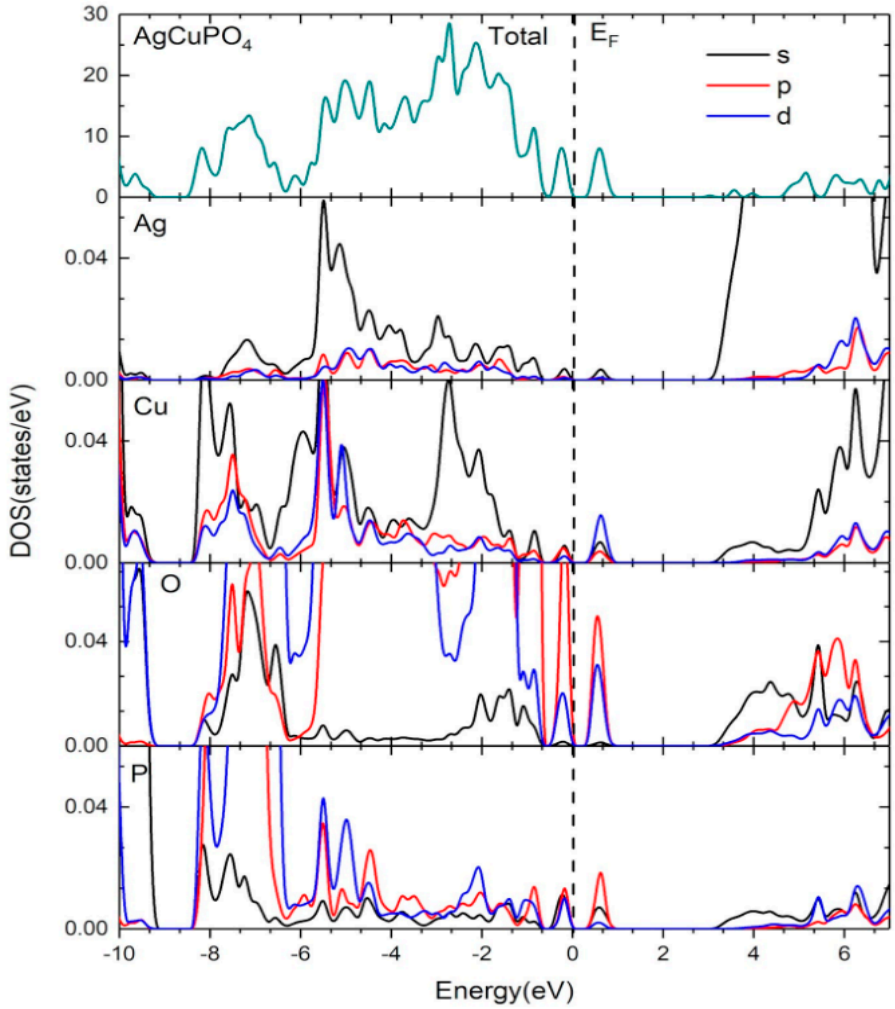

Figure S3. Calculated total and site projected density of states of $AgCuPO_4$. The Fermi level is set to zero and marked by a vertical dotted line.

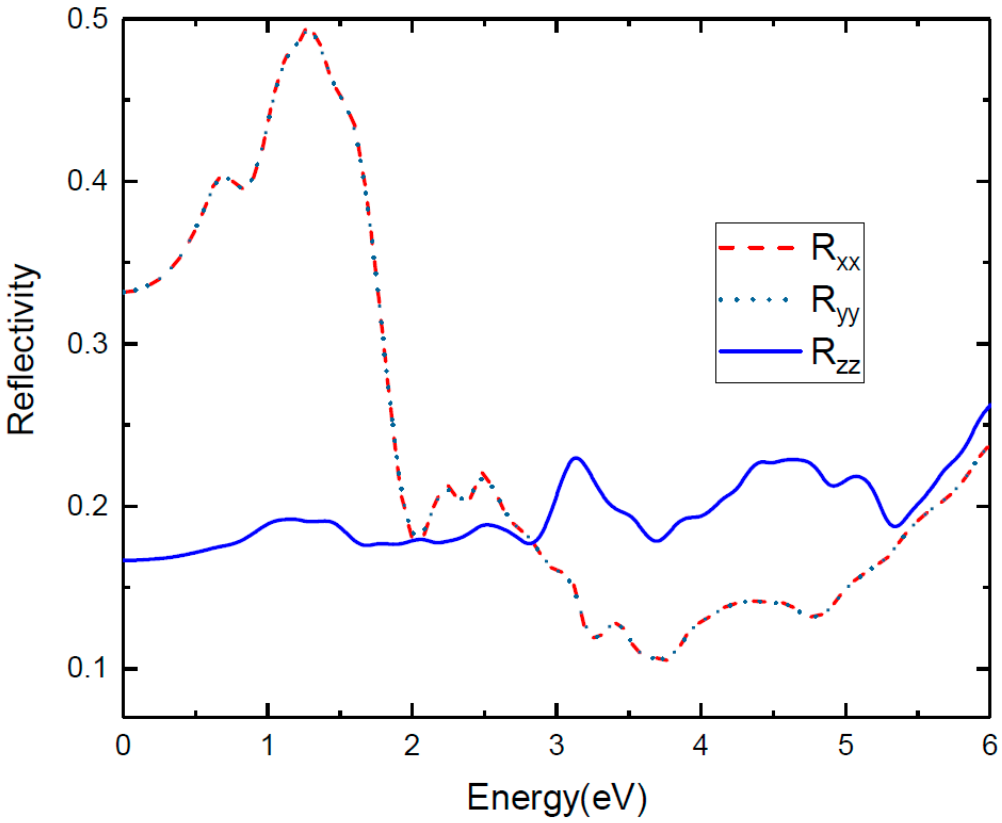

Figure S4. Reflectivity of $Au_2Cs_2I_6$ along x, y and z directions.

In the quest of an efficient photovoltaic material, its optical reflectivity plays also vital role. We present results from our study in which first principle calculation is carried out employing hybrid functional HSE06 to calculate the optical reflectivity of the materials of interest. In Fig. S4, we show reflectivity of $Au_2Cs_2I_6$ as function of photon energy in all directions. As compared to other three compounds, anisotropy is more pronounced in $Au_2Cs_2I_6$. We notice that the reflectivity is 0.35 – 0.5 in the infrared region and the value drops in the high energy region along *x* and *y* directions. In the *z*-direction, we notice that the reflectivity is 0.185 in the infrared region and 0.165-0.24 in the visible region with some peaks. It is also noticed that the reflectivity of $Au_2Cs_2I_6$ is less in visible region, which indicates $Au_2Cs_2I_6$ can be used as photovoltaic applications.

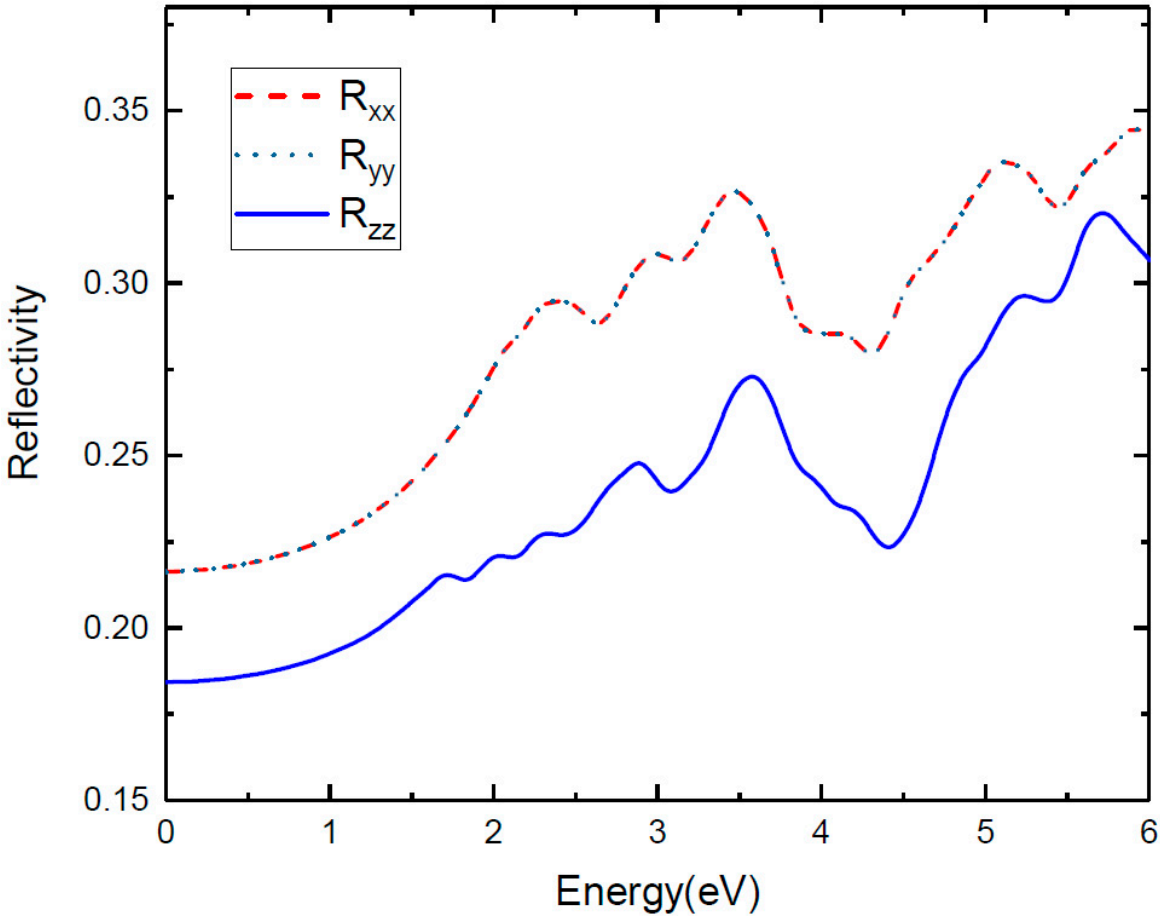

Figure S5. Reflectivity of Ag_2GeBaS_4 along x, y and z directions.

We show reflectivity of Ag_2GeBaS_4 as function of photon energy in *x*, *y* and *z* directions in the Fig.S5. We notice that the reflectivity 0.165 – 0.24 present in the infrared region and low-energy of visible region along *z*-direction. At 3 eV, the reflectivity drops by small values and then the value increases in the high energy region along *z*-direction. In *x* and *y* direction, we notice that the reflectivity 0.22-0.32 present in the infrared region and visible region with some peaks. It is also noticed that the reflectivity of Ag_2GeBaS_4 is little high in visible region along *x*, *y* and *z* directions.

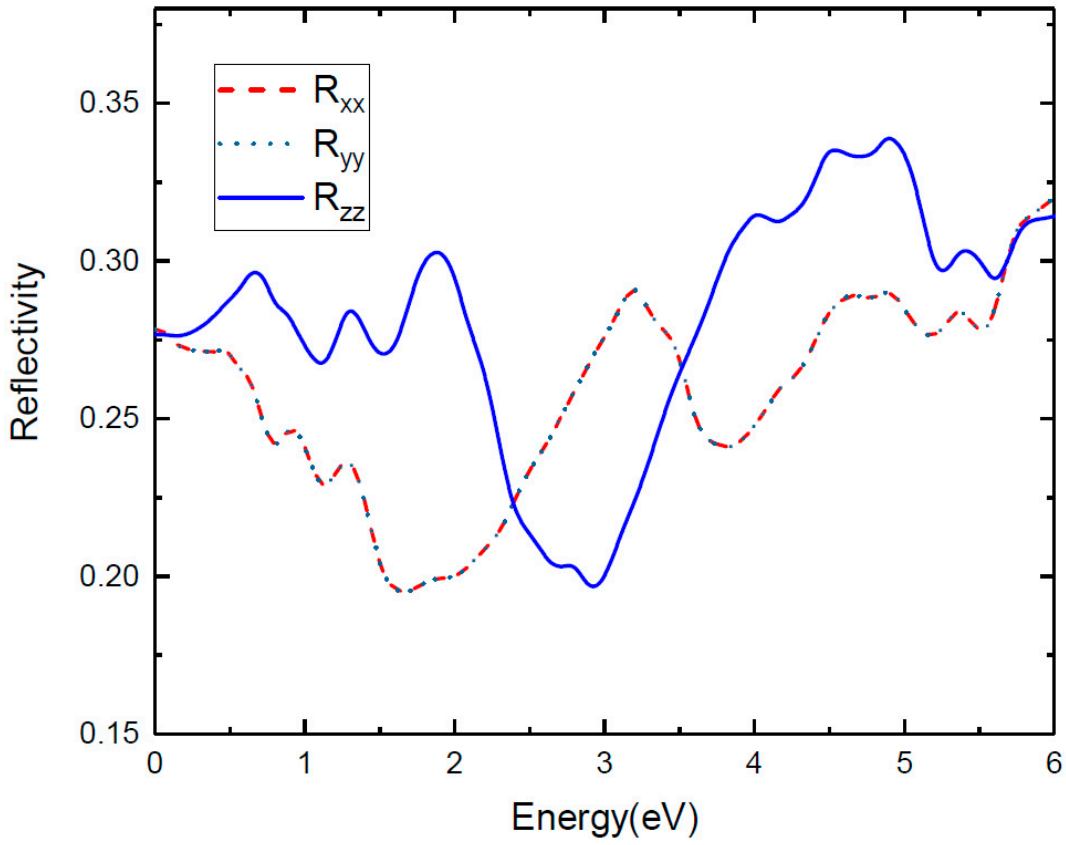

Figure S6. Reflectivity of Ag_2ZnSnS_4 along x, y and z directions.

The reflectivity of Ag_2ZnSnS_4 is high at 0.6 and 2 eV photon energy and very low at 3 eV photon energy for *z*-direction as shown in Fig.S6. However, the reflectivity is very low at 1.5 – 2 eV along *x* and *y* directions, which indicates this material, can be used as photovoltaic applications.

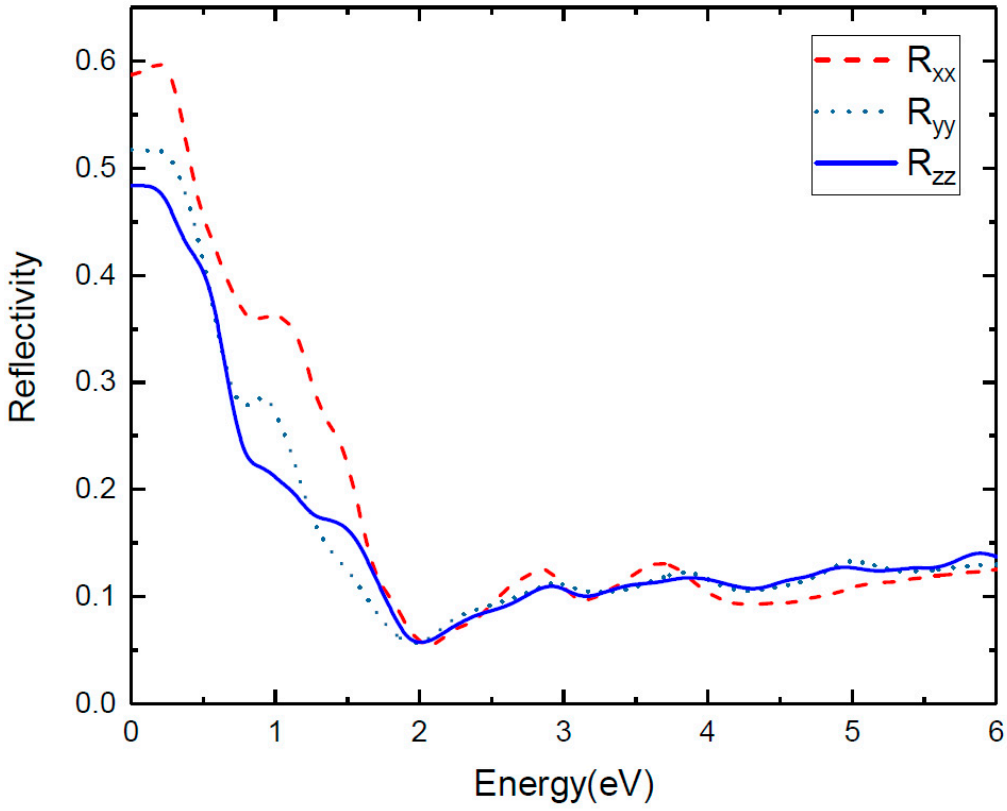

Figure S7. Reflectivity of $AgCuPO_4$ along x, y and z directions.

In Fig. S7, we show reflectivity of the $AgCuPO_4$ as function of photon energy in all direction. We notice that the reflectivity 0.1–0.59 present in the infrared region and the value drops in the visible region along *x*, *y* and *z* directions. It is also noticed that the reflectivity of $AgCuPO_4$ is less in visible region in all directions, which indicates this material can be used as photovoltaic applications. From the imaginary part of the dielectric function, absorption coefficients and electronic band structures, we can conclude that all four compounds exhibit three-level optical transitions. This will lead to enhanced light absorption in the extended visible region.