**Exploring Double Perovskites Cs2AgSbX6 (X = Cl, Br, I) as Promising Optoelectronic and Thermoelectric Materials: A First-Principles Study**

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1. **Spectroscopic Limited Maximum efficiency Model**

The spectroscopic limited maximum efficiency (SLME) approach, introduced by Yu and Zunger,[1](#_ENREF_1) is employed to assess the theoretical efficiency of semiconductors. This method generalizes the widely recognized Shockley–Queisser (SQ) criterion for determining the maximum efficiency of an absorber layer.[2](#_ENREF_2) In this model the photoelectric conversion efficiency is expressed as:

ɳ 1

Here, ɳ represents the photoelectric conversion efficiency, is the output power and denote input power, respectively. The output power is determined by the open-circuit voltage Voc and the current density *J*. It is given by:

2

Where is the short-circuit current density, is the reverse saturation current density (or total electron-hole recombination current) and k*B* is the [Boltzmann constant](https://www.sciencedirect.com/topics/engineering/boltzmanns-constant). and are defined as

3

4

In these expressions stands for the absorption coefficient, is the length of the absorber layer, is standard AM1.5G sun spectrum, represents the blackbody spectrum at temperature T, and is the radiative recombination fraction, calculated as:

5

The open-circuit voltage , which represents the voltage at zero current density, is given by:

6

The fill factor FF is computed as:

7

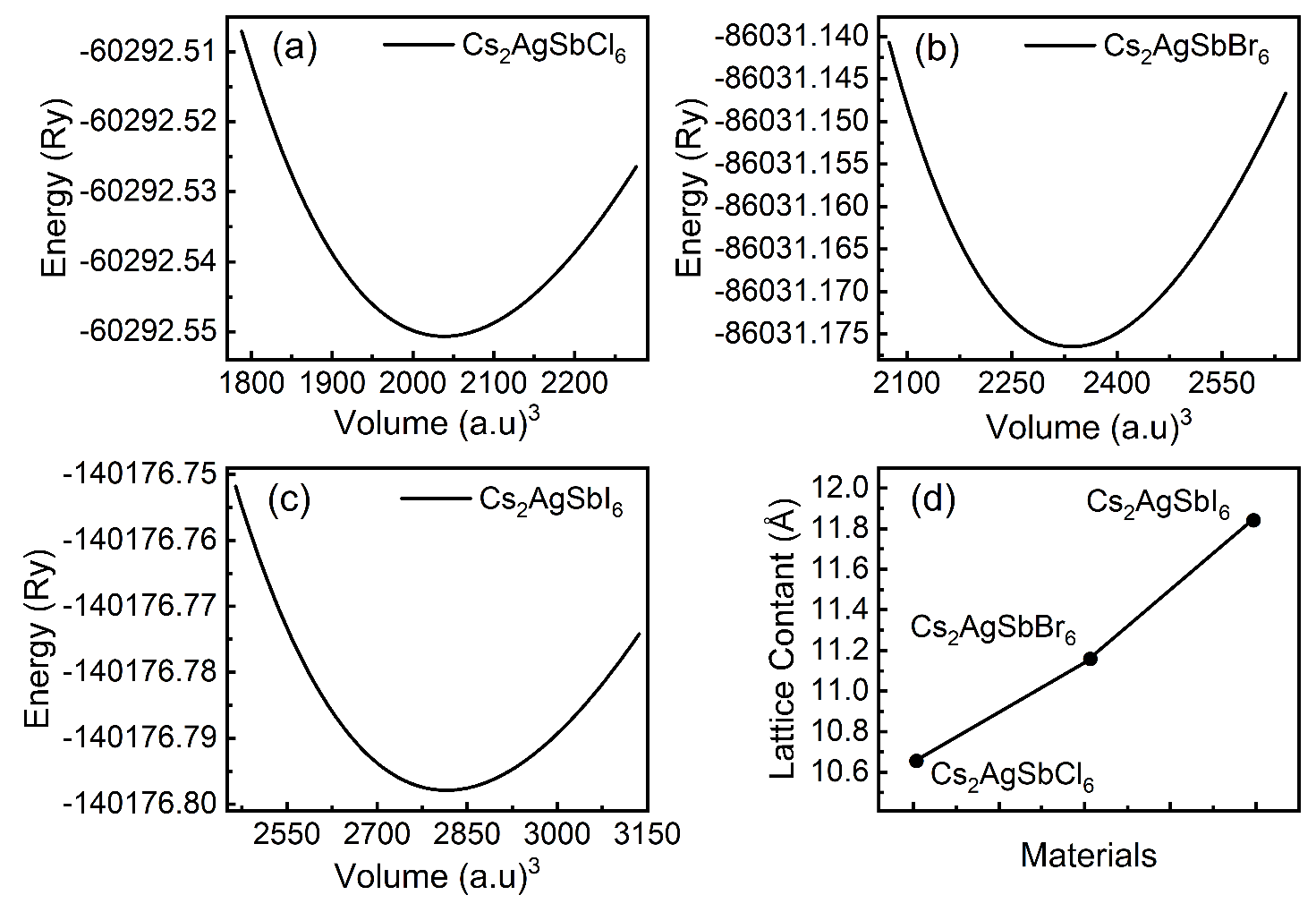
The input density can be obtained as

8

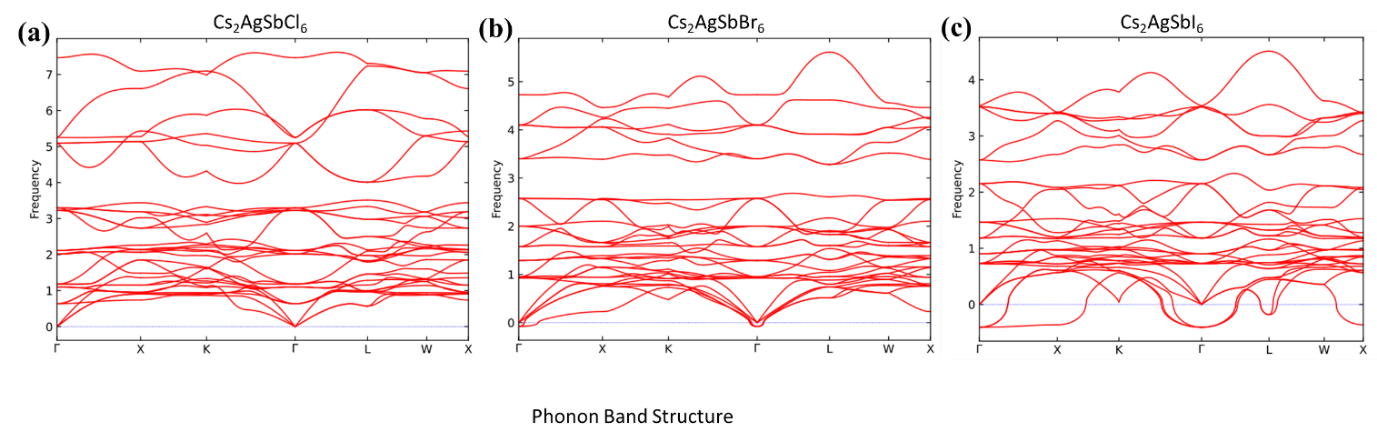
Where E is the photon energy.

Finally, the maximum photovoltaic conversion efficiency of the absorber layer is calculated as:

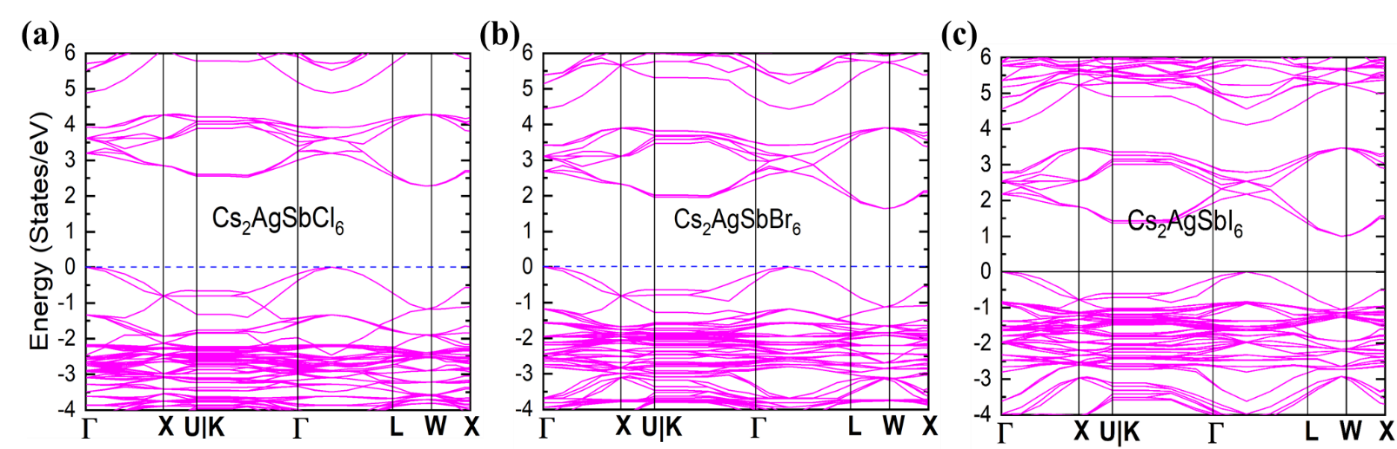
ɳ 9



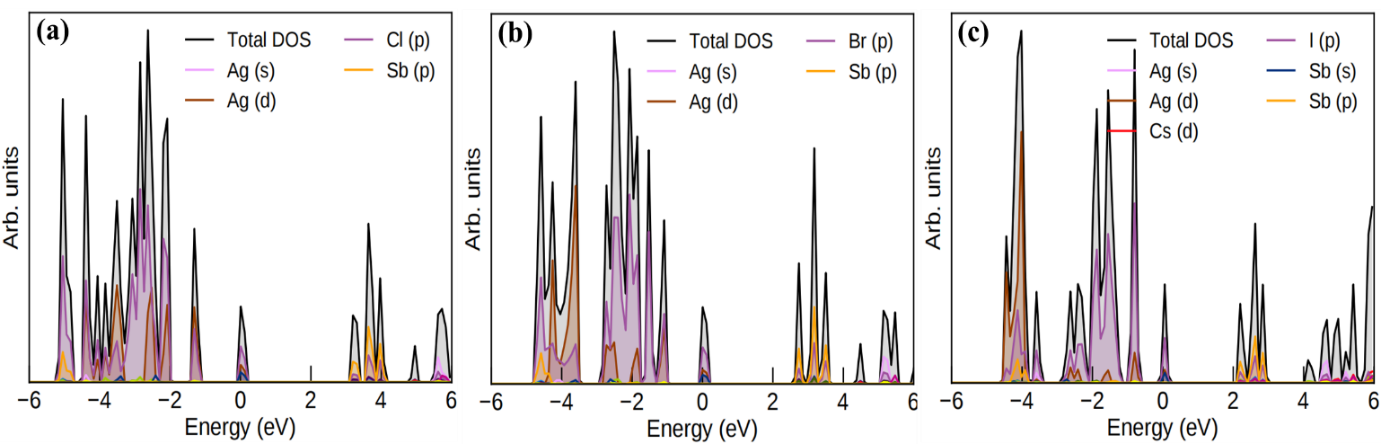
**Figure S1.** (a-c)Volume optimization results for Cs2AgSbX6 (Cl, Br, I), (d) Variation of lattice constant with halogens (Cl, Br, I).



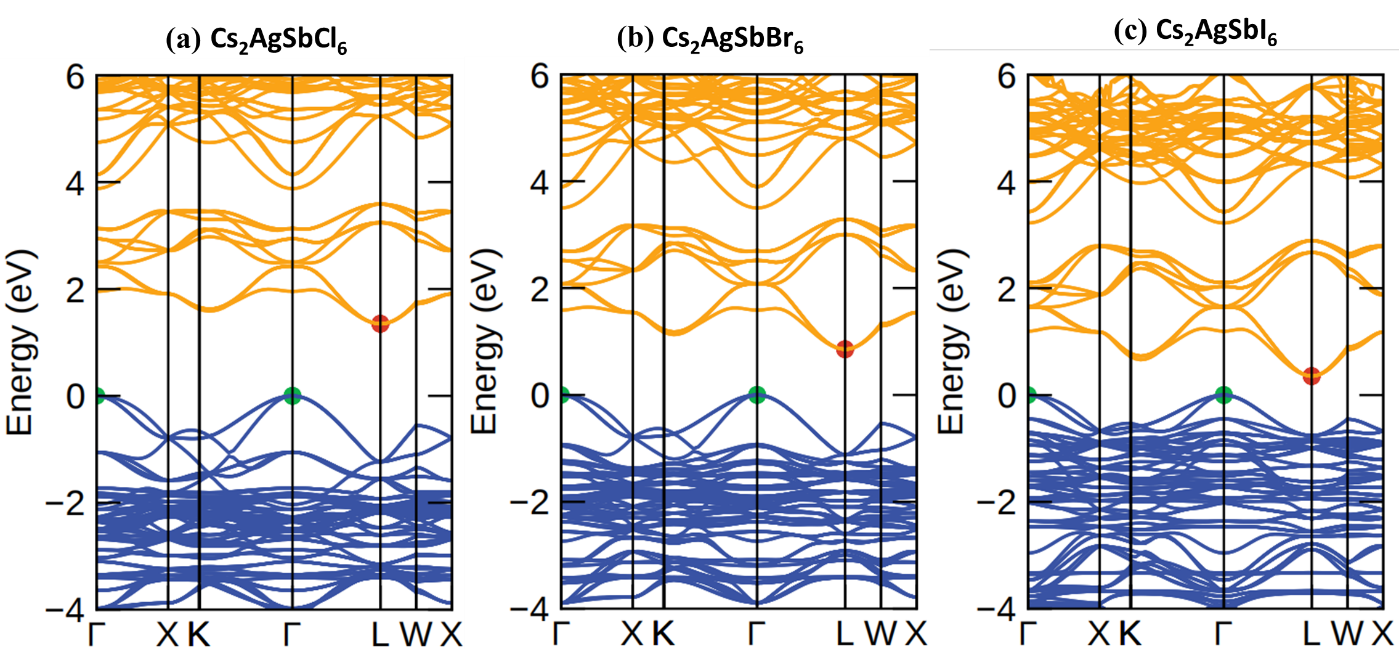
**Figure S2.** Phonon band structure at 0 Kfor Cs2AgSbX6 (X= Cl, Br, I).



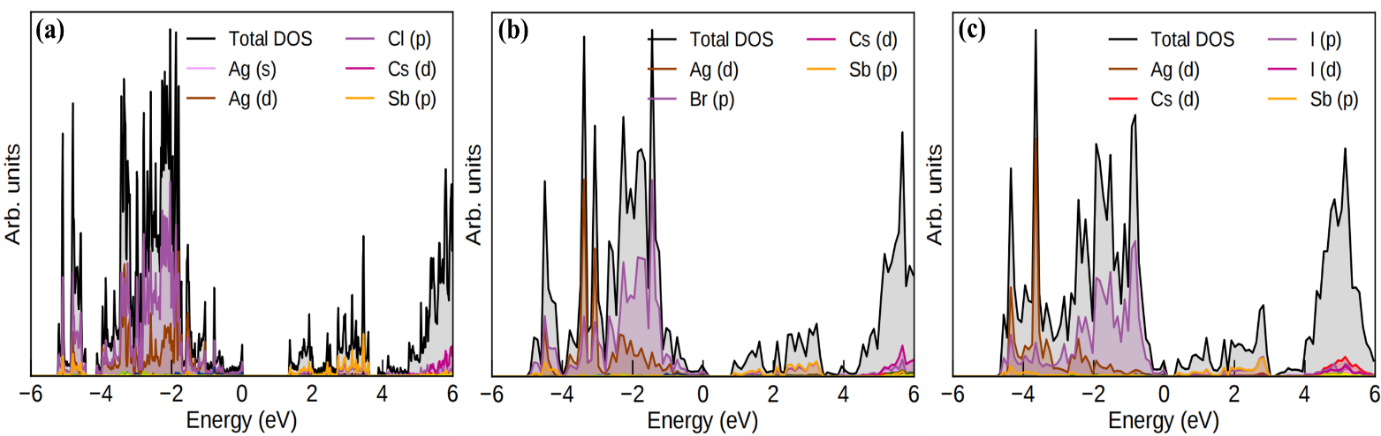
**Figure S3.** Band structure via HSE06 functional.



**Figure S4.** HSE calculated DOS of Cs2AgSbX6 (X=Cl, Br, I).



**Figure S5.** Band structure via PBE-SOC.



**Figure S6**: Calculated DOS of Cs2AgSbX6 (X=Cl, Br, I) using PBE-SOC method.

1. Yu, L.; Zunger, A., Identification of Potential Photovoltaic Absorbers Based on First-Principles<? format?> Spectroscopic Screening of Materials. *Physical review letters* **2012,** *108* (6), 068701.

2. Shockley, W.; Queisser, H., Detailed balance limit of efficiency of p–n junction solar cells. In *Renewable energy*, Routledge: 2018; pp Vol2\_35-Vol2\_54.