Thermoelectric Properties of doped-Cu_3SbSe_4 compounds: A First-principles Insight

Gregorio Garcia,[1,2] Pablo Palacios,[1,3*] Andreu Cabot,[4,5] Perla Wahnón[1,2]

[1] Instituto de Energia Solar, ETSI Telecomunicación, Universidad Politécnica de Madrid, Ciudad Universitaria, s/n, 28040, Madrid, Spain

[2] Departamento de Tecnologia Fotónica y Bioingenieria, ETSI Telecomunicación, Universidad Politécnica de Madrid, Ciudad Universitaria, s/n, 28040 Madrid, Spain

[3] Departamento de Fisica aplicada a las Ingenierías Aeronáutica y Naval. ETSI Aeronáutica y del Espacio, Universidad Politécnica de Madrid, Pz. Cardenal Cisneros, 3, 28040 Madrid, Spain.

[4] Catalonia Institute for Energy Research - IREC, 08930 Sant Adrià de Besòs, Barcelona, Spain.

[5] ICREA, Pg. Lluis Companys, 23, 08010 Barcelona, Spain.

* Corresponding author: pablo.palacios@upm.es (P.P.)

SUPLEMENTARY INFORMATION

Table S1. Crystal structure of Sb and M (M = Al, Ga, In, Tl, Si, Ge, Sn, Pb, P, As, Bi) atoms.

Atom	Space Group	Cell axis / Å	Reference
Sb	166	$a = b = 4.61$ $c = 11.27$	Review of Scientific Instruments, 1977, 48, 24
M			
Al	225	$a = b = c = 4.05$	Acta Crystallographica, 1962,15, 578
Ga	64	$a = 4.51$ $b = 7.66$ $c = 4.52$	Z. Kristallogr. Kristallgeom. Kristallphys. Kristallchem., 1962, 117, 293
In	139	$a = b = 3.25$ $c = 4.87$	Physical Review, 1921, 17, 266
Tl	194	$a = b = 3.45$ $c = 5.52$	Physical Review, 1958, 110, 1071
Si	227	$a = b = c = 5.43$	Physica Status Solidi, 1962, 2, 984
Ge	225	$a = b = c = 5.66$	Acta Crystallographica, 1962, 15, 578
Sn	141	$a = b = 5.83$ $c = 3.18$	Acta Crystallographica,1961, 14, 355
Pb	225	$a = b = c = 4.92$	Philosophical Magazine, 1916, 32, 65
P	2	$a = 11.45$ $b = 5.50$ $c = 11.26$	Phosphorus and Sulfur and the Related Elements, 1987, 30, 507
As	166	$a = b = 3.76$ $c = 10.44$	Journal of Applied Crystallography, 1969, 2, 30 36
Bi	166	$a = b = 4.55$ $c = 11.86$	Acta Crystallographica, 1962, 15, 865

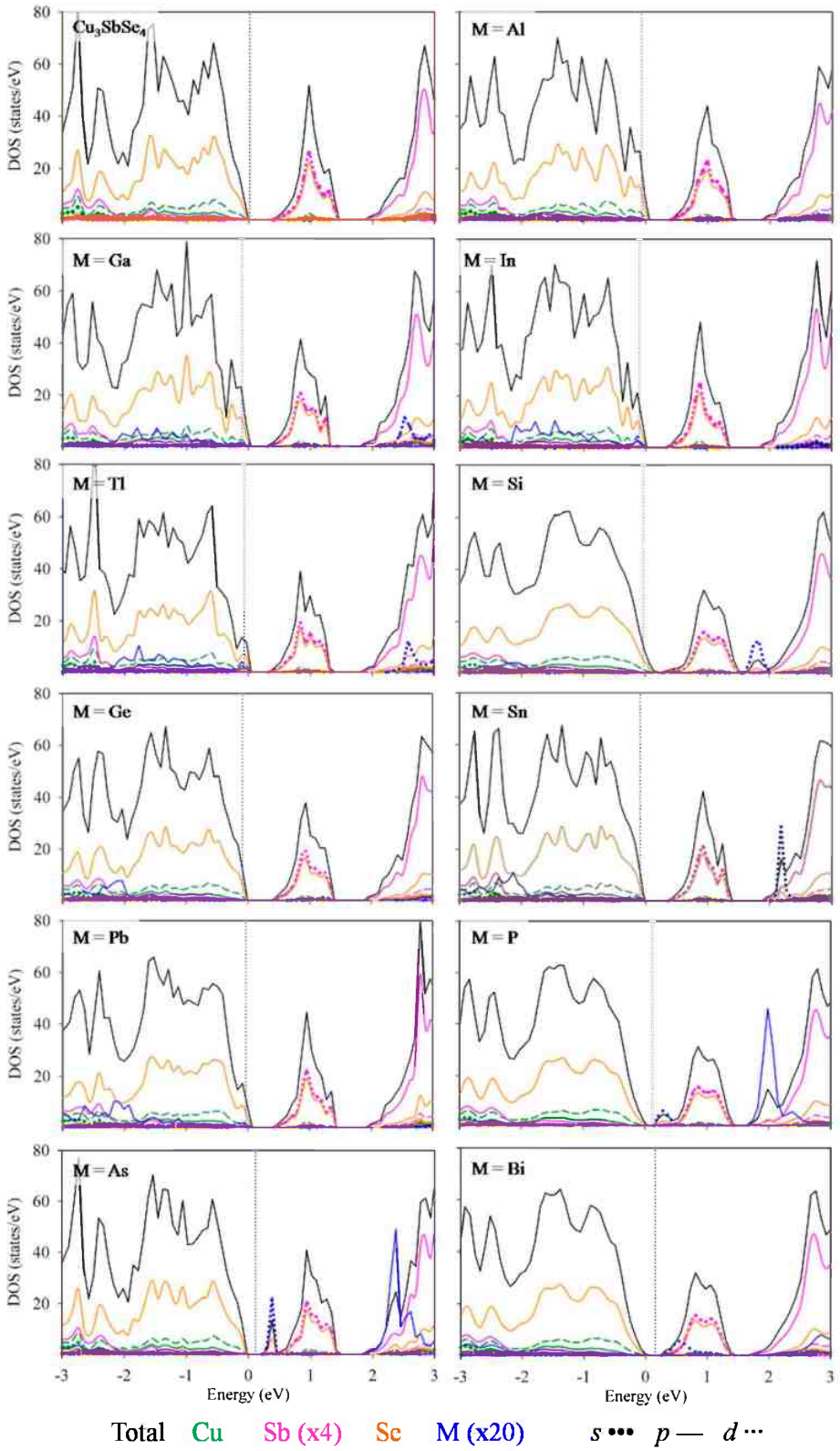

Figure S1. Projected Density of States of Cu_3SbSe_4 and $Cu_3Sb_{1-x}M_xSe_4$ (M = Al, Ga, In, Tl, Si, Ge, Sn, Pb, P, As and Bi) compounds. The zero of energy has been set at the valence band energy, while blue dotted line represents the Fermi level (E_{Fermi}).

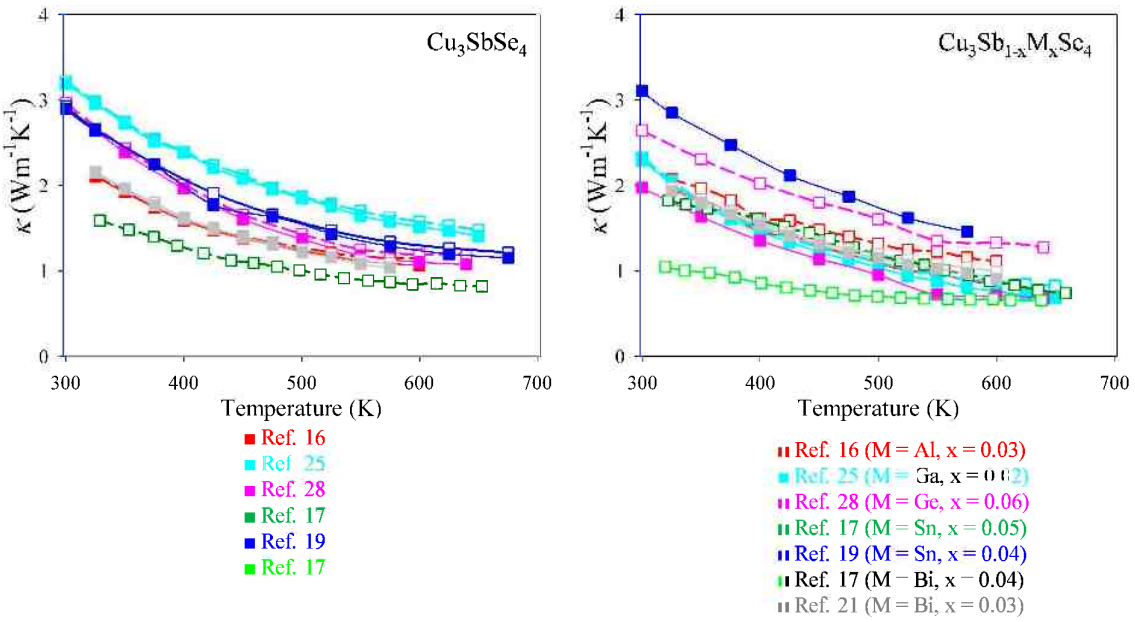

Figure S2. Summary of experimental data for the total thermal conductivity (unfilled symbols) and lattice contribution (filled symbols) for holes of Cu_3SbSe_4 and $Cu_3Sb_{1-x}M_xSe_4$ (M = Al, Ga, Ge, Sn, Bi) compounds.