Supplementary Material: Chalcogenide Perovskite $YScS_3$ as a potential p-Type Transparent Conducting Material

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The CIF file for the optimized structure of $YScS_3$ in perovskite structure

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_cell_length_b    9.5258
_cell_length_c    6.3716
_cell_angle_alpha 90.
_cell_angle_beta  90.
_cell_angle_gamma 90.

_symmetry_space_group_name_H-M "P 21/n 21/m 21/a"
_symmetry_Int_Tables_number 62
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_space_group.transform_Pp_abc a,b,c;0,0,0

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_space_group_symop_operation_xyz
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3 -x,y+1/2,-z
4 -x+1/2,-y,z+1/2
5 -x,-y,-z
6 -x+1/2,y+1/2,z+1/2
7 x,-y+1/2,z
8 x+1/2,y,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Y1  Y    4 c 0.40087 0.25000 0.04004 1.00000
Sc1 Sc   4 a 0.00000 0.00000 0.00000 1.00000
S1  S    4 c 0.04892 0.25000 0.85653 1.00000
S2  S    8 d 0.68506 0.42882 0.17658 1.00000
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The CIF file for optimized structure of $YScS_3$ in $UFeS_3$ structure

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_cell_angle_gamma 90.

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_symmetry_Int_Tables_number 63
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_space_group.transform_Pp_abc a,b,c;0,0,0

loop_
_space_group_symop_id
_space_group_symop_operation_xyz
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2 x,-y,-z
3 -x,y,-z+1/2
4 -x,-y,z+1/2
5 -x,-y,-z
6 -x,y,z
7 x,-y,z+1/2
8 x,y,-z+1/2
9 x+1/2,y+1/2,z
10 x+1/2,-y+1/2,-z
11 -x+1/2,y+1/2,-z+1/2
12 -x+1/2,-y+1/2,z+1/2
13 -x+1/2,-y+1/2,-z
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16 x+1/2,y+1/2,-z+1/2

loop_
_atom_site_label
_atom_site_type_symbol
_atom_site_symmetry_multiplicity
_atom_site_Wyckoff_label
_atom_site_fract_x
_atom_site_fract_y
_atom_site_fract_z
_atom_site_occupancy
Y1  Y    4 c 0.00000 0.25275  0.25000 1.00000
Sc1 Sc   4 a 0.00000 0.00000  0.00000 1.00000
S1  S    4 c 0.00000 -0.08586 0.25000 1.00000
S2  S    8 f 0.00000 0.35849  0.56369 1.00000
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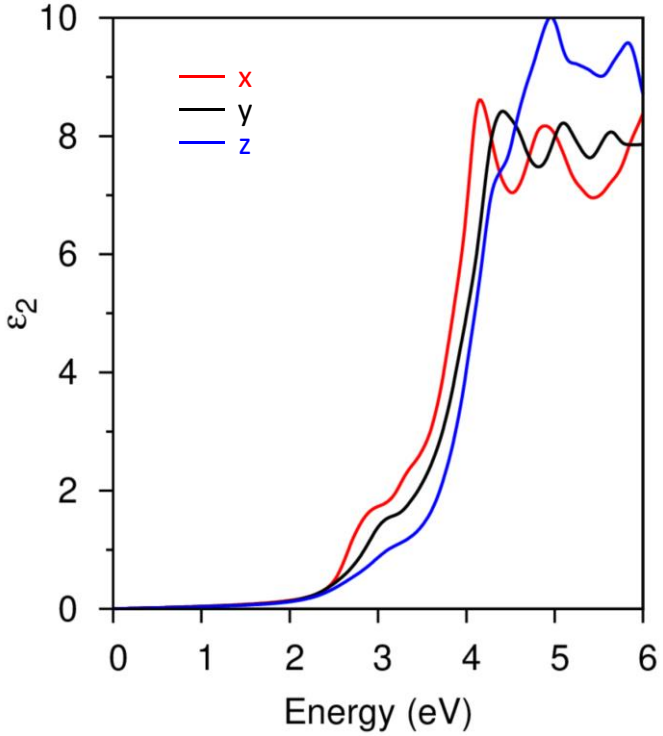

Figure S1. Imaginary part of dielectric constant (ε_2) of $YScS_3$ in the $UFeS_3$ structure.

Table S1. The hole effective mass of potential p-type transparent conducting materials. The unit is m_0. The values of m_h^1, m_h^2 and m_h^3 were collected from a computational electronic transport database,[1] which was generated using PBE functional without considering spin-orbit coupling (SOC) effect. The conductivity effective mass m_c was calculated according to the formula shown in the main text. It can be seen that none of these materials exhibit m_c smaller than 0.5 m_0.

	m_h^1	m_h^2	m_h^3	m_c
AlN	0.43	3.58	3.58	1.04
GaN	1.56	1.56	1.85	1.65
ZnO	1.85	1.85	2.96	2.11
ZnS	1.07	1.07	1.61	1.20
In_2O_3	6.05	6.05	6.05	6.05
SnO_2	1.47	1.47	2.11	1.64
$CuAlO_2$	1.92	1.92	5.22	2.43
$CuAlS_2$	1.02	1.76	1.76	1.42
$CuGaO_2$	2.46	2.46	5.00	2.96
CuI	0.86	0.86	0.86	0.86
BaCuSeF	0.69	0.69	253	1.03
BaCuTeF	0.52	0.52	137	0.78
Al_2Se_3	0.64	0.69	308	1.00
MgS	0.98	0.98	0.98	0.98
MgSe	1.24	1.24	1.24	1.24
MgTe	1.31	1.71	1.71	1.55

[1] F. Ricci, W. Chen, U. Aydemir, G. J. Snyder, G.-M. Rignanese, A. Jain, and G. Hautier, Scientific Data **4,** 170085 (2017).

Table S2. Calculated formation energy of p-type dopants at Y and Sc sites in neutral charge state using the SCAN functional. The unit is eV.

	Mg	Ca	Sr	Ba	Zn
On Y site	1.11	0.78	0.66	0.87	1.35
On Sc site	0.73	1.37	2.06	3.19	1.34