Supporting Information for "First principles based screen for identification of transparent conductors"

Yuwei Li[†,‡] and David J. Singh[*,‡]

North China Institute of Aerospace Engineering, No. 133 Aimin East Road , Langfang, Hebei 065000, China, and Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211-7010 USA

E-mail: singhdj@missouri.edu

[*]To whom correspondence should be addressed
[†]North China Institute of Aerospace Engineering, No. 133 Aimin East Road , Langfang, Hebei 065000, China
[‡]Department of Physics and Astronomy, University of Missouri, Columbia, MO 65211-7010 USA

Table S1: The optical and electrical fitness function (OEF) of the wide bandgap semiconductors considered. All materials are calculated for p-type, except In_2O_3, which is shown for n-type.

	OEF			
	solar		PV	
	10^{20} cm^{-3}	10^{21} cm^{-3}	10^{20} cm^{-3}	10^{21} cm^{-3}
BP	12.47	14.93	16.98	21.18
ZnS	13.01	14.61	17.73	20.61
MgS	11.95	14.35	16.26	20.56
MgTe	14.38	13.36	18.50	21.20
B_6O	12.44	13.17	16.90	19.30
ZnSe	13.03	12.07	8.56	20.50
BeTe	13.89	11.36	18.69	20.51
La_2O_2Te	6.52	11.24	0.24	8.38
GaSe	8.14	10.92	2.51	14.83
ZnTe	9.35	8.91	1.02	18.18
Al_2Se_3	7.34	8.28	9.97	10.71
Ba_2BiTaO_6	10.24	8.07	12.55	9.68
$CsLaO_2$	7.46	7.87	13.36	16.43
$AgLaO_2$	5.85	7.11	6.89	9.53
La_2O_2Se	6.56	6.41	6.76	6.40
$BrLaO_2$	6.17	6.25	8.54	8.36
$AgYS_2$	4.31	5.54	0.24	4.79
$Cs_2Zn_3Te_4$	5.61	5.42	2.54	7.15
$CuAlO_2$	5.23	5.31	4.81	4.73
$AgAlO_2$	4.57	4.96	0.22	1.45
KYS_2	6.00	4.76	14.10	12.99
$Cs_2Zn_3Se_4$	4.95	4.68	6.44	4.18
$CaPb_2O_3$	3.77	3.79	5.37	5.76
$SrPb_2O_3$	3.33	2.71	4.26	3.67
$BaPbO_2$	2.98	2.62	4.02	3.93
Pr_2SeO_2	1.20	2.60	0.11	0.69
$BaPb_2O_3$	2.09	1.96	2.51	2.45
In_2O_3	14.40	14.78	20.27	20.85

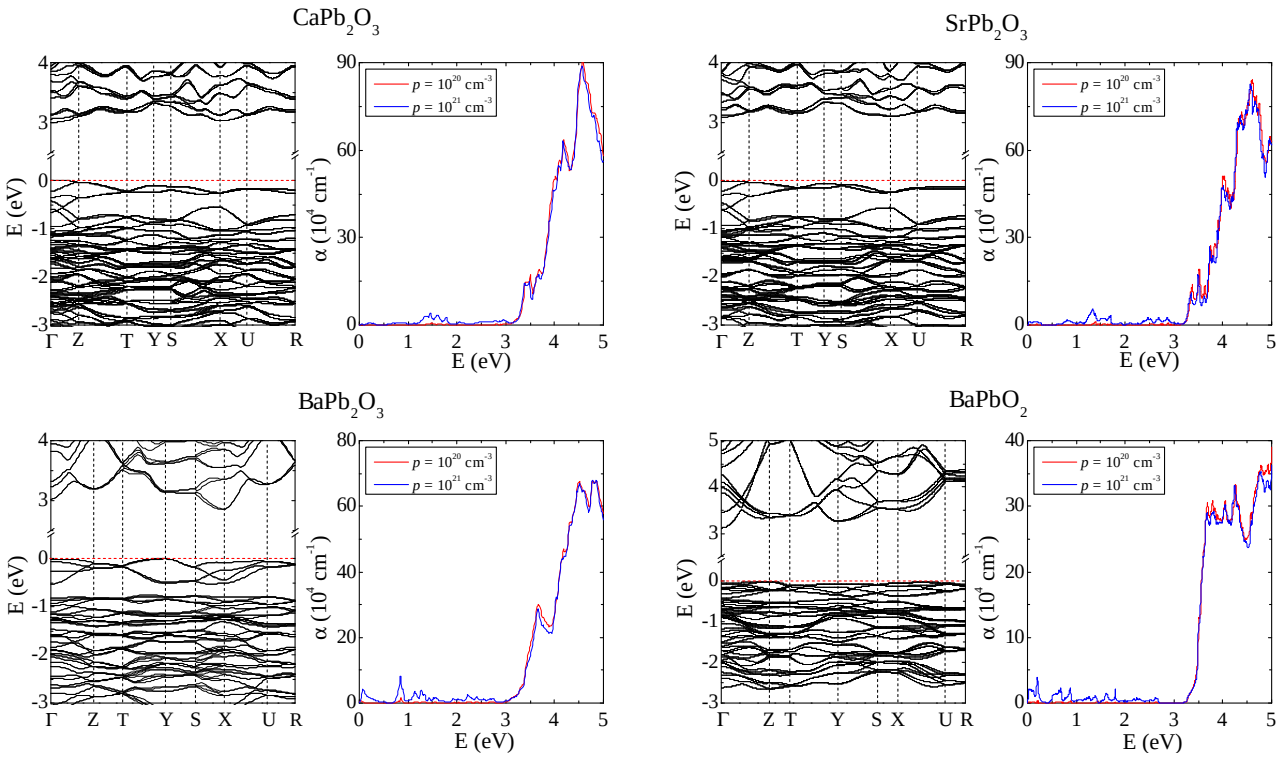

Figure S1: The band structures and absorption spectra of $CaPb_2O_3$, $SrPb_2O_3$, $BaPb_2O_3$ and $BaPbO_2$ respectively. The valence band maximum is set to energy zero.

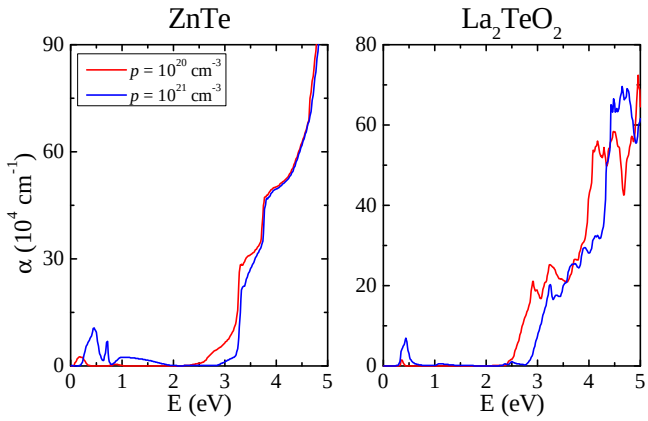

Figure S2: The absorption spectra of ZnTe and La_2TeO_2 respectively.

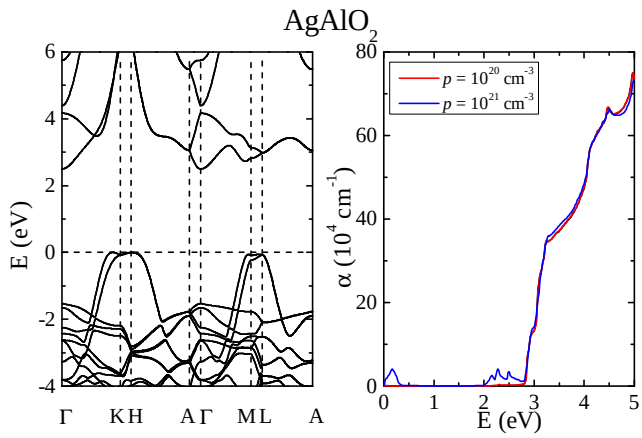

Figure S3: The band structure and absorption spectrum of $AgAlO_2$. The valence band maximum is set to energy zero.

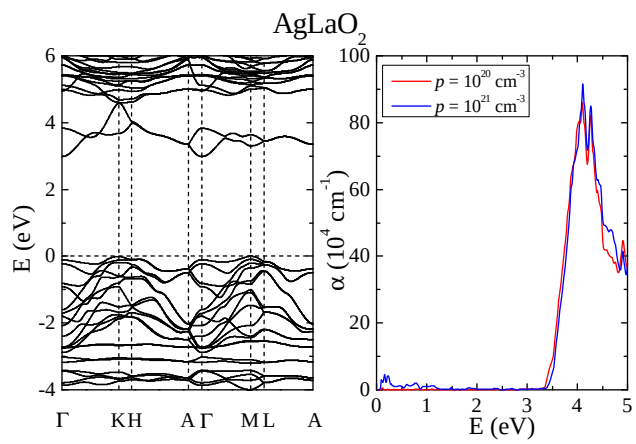

Figure S4: The band structure and absorption spectrum of $AgLaO_2$. The valence band maximum is set to energy zero.

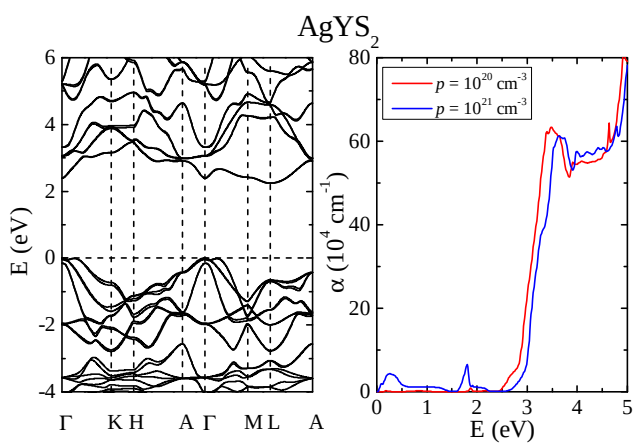

Figure S5: The band structure and absorption spectrum of $AgYS_2$. The valence band maximum is set to energy zero.

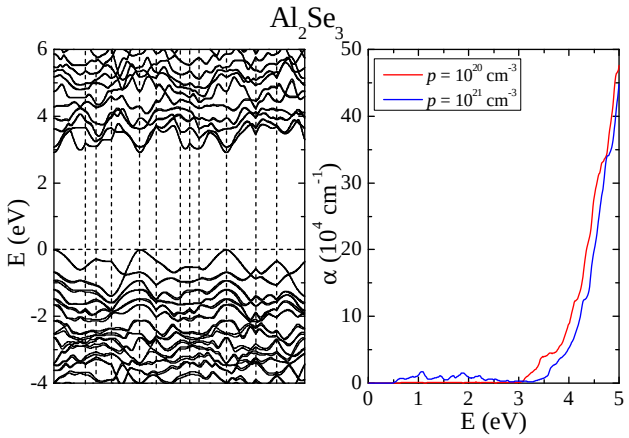

Figure S6: The band structure and absorption spectrum of Al_2Se_3. The valence band maximum is set to energy zero. Band structure path: (0.00, 0.00, 0.00) - (0.50, 0.00, 0.00) - (0.54, -0.04, 0.26) - (0.40, -0.04, 0.40) - (0.00, 0.00, 0.00) - (-0.10, 0.64, -0.10) - (0.40, 0.23, -0.00) - (0.50, -0.00, -0.00) - (0.63, -0.27, 0.27) - (0.00, 0.00, 0.00) - (0.27, 0.50, -0.27) - (-0.10, 0.64, -0.10) - (0.40, -0.04, 0.40).

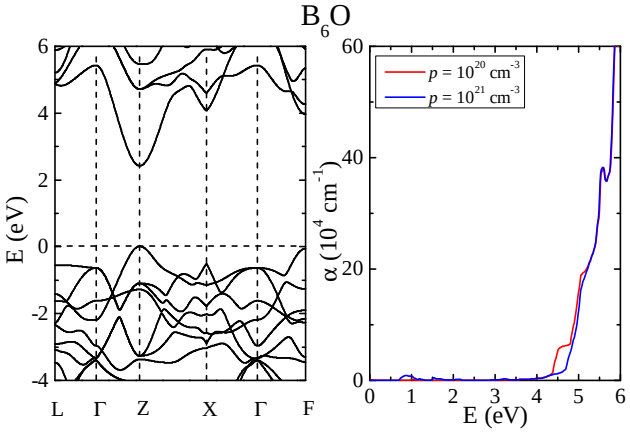

Figure S7: The band structure and absorption spectrum of B_6O. The valence band maximum is set to energy zero.

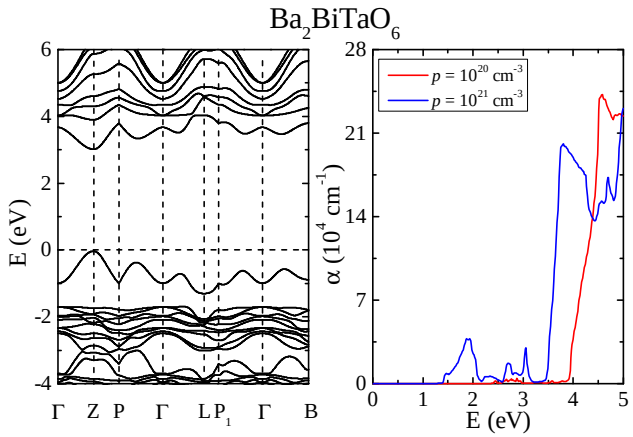

Figure S8: The band structure and absorption spectrum of Ba_2BiTaO_6. The valence band maximum is set to energy zero.

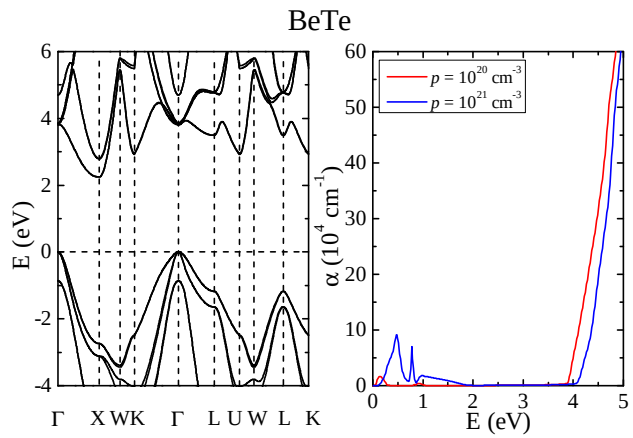

Figure S9: The band structure and absorption spectrum of BeTe. The valence band maximum is set to energy zero.

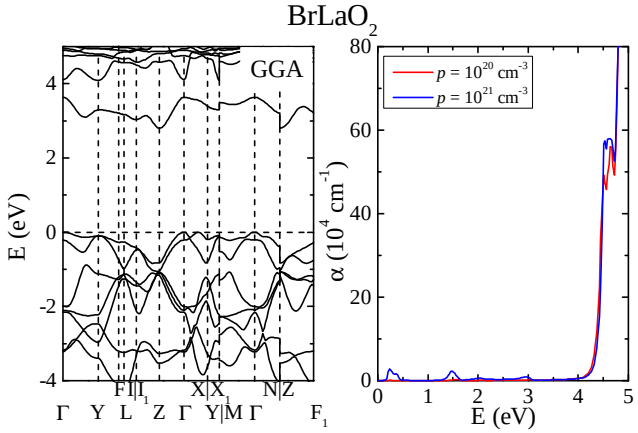

Figure S10: The band structure and absorption spectrum of $BrLaO_2$. The band structure is calculated using VASP code with the generalized gradient approximation of Perdew, Burke and Ernzerhof (PBE-GGA). The valence band maximum is set to energy zero.

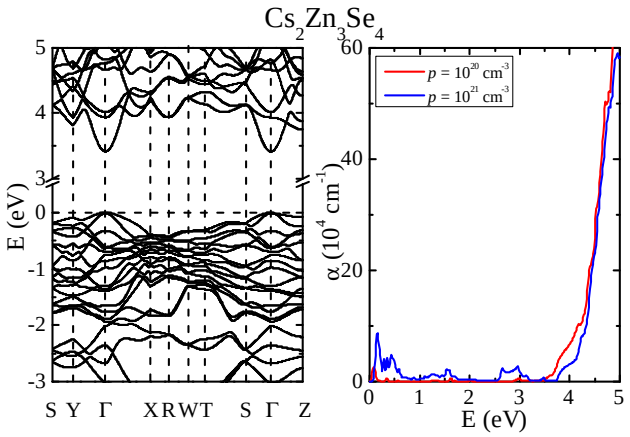

Figure S11: The band structure and absorption spectrum of $Cs_2Zn_3Se_4$. The valence band maximum is set to energy zero.

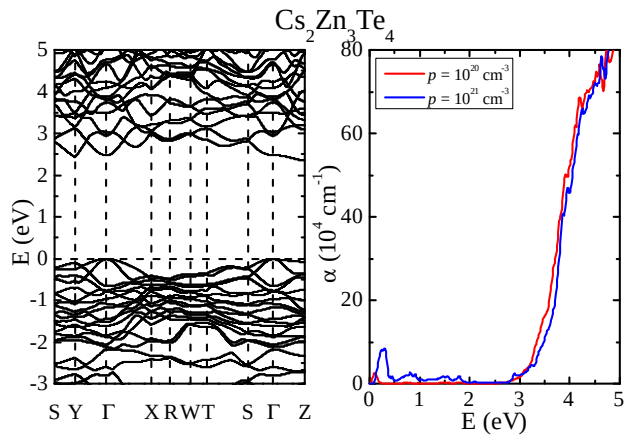

Figure S12: The band structure and absorption spectrum of $Cs_2Zn_3Te_4$. The valence band maximum is set to energy zero.

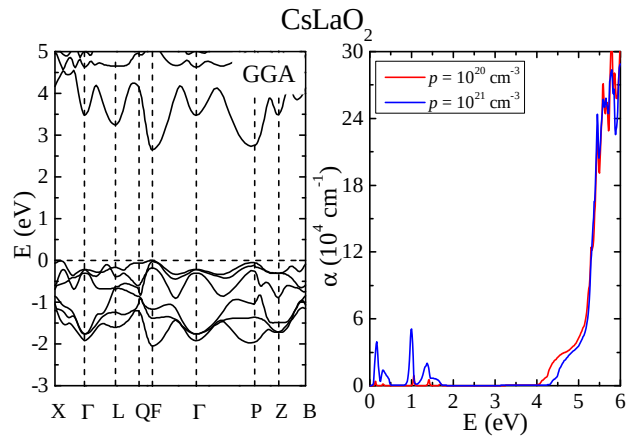

Figure S13: The band structure and absorption spectrum of $CsLaO_2$. The band structure is calculated using VASP code with the PBE-GGA functional. The valence band maximum is set to energy zero.

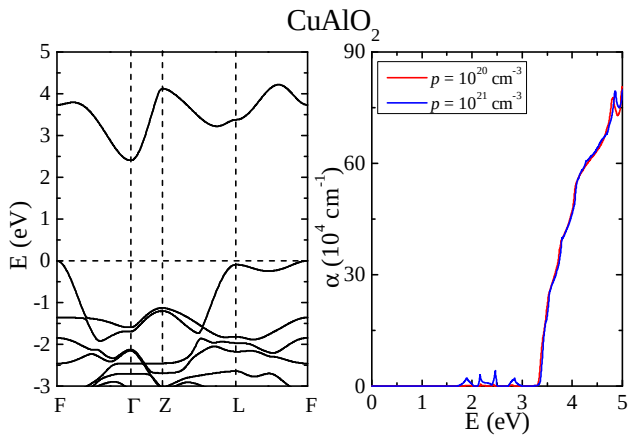

Figure S14: The band structure and absorption spectrum of $CuAlO_2$. The valence band maximum is set to energy zero.

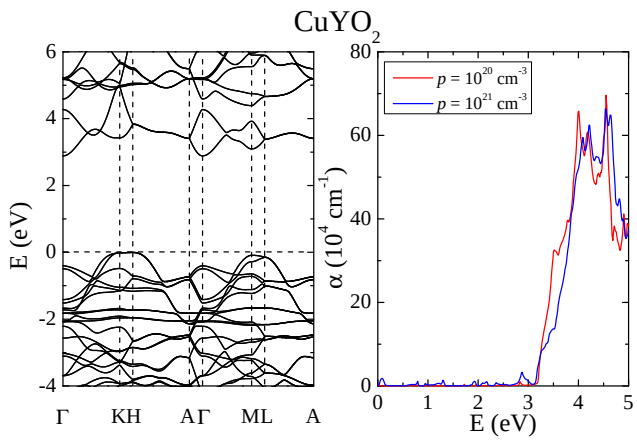

Figure S15: The band structure and absorption spectrum of $CuYO_2$. The valence band maximum is set to energy zero.

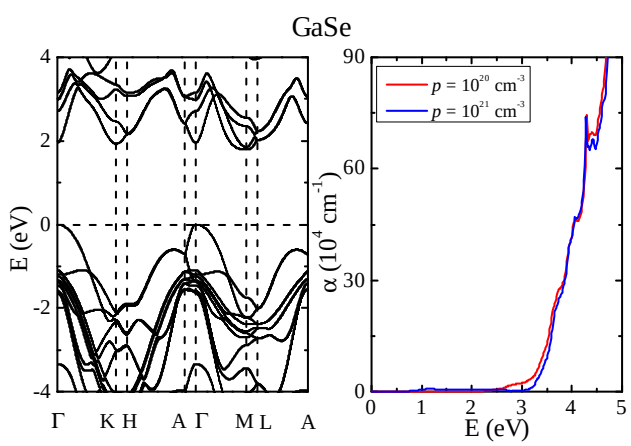

Figure S16: The band structure and absorption spectrum of GaSe. The valence band maximum is set to energy zero.

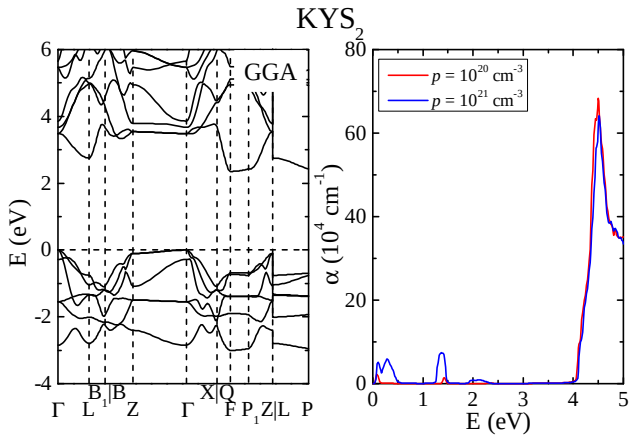

Figure S17: The band structure and absorption spectrum of KYS_2. The band structure is calculated using VASP code with the PBE-GGA functional. The valence band maximum is set to energy zero.

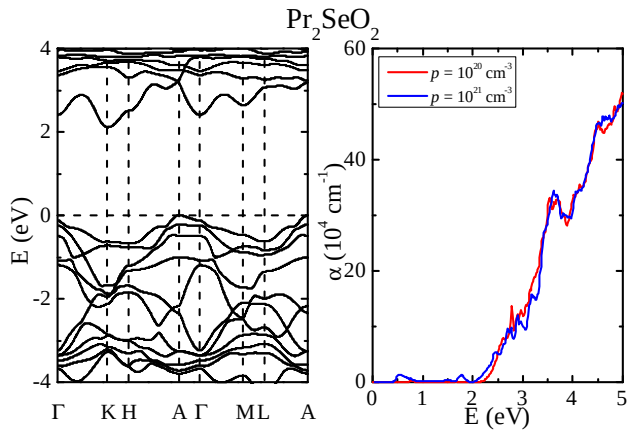

Figure S18: The band structure and absorption spectrum of Pr_2SeO_2. The valence band maximum is set to energy zero.

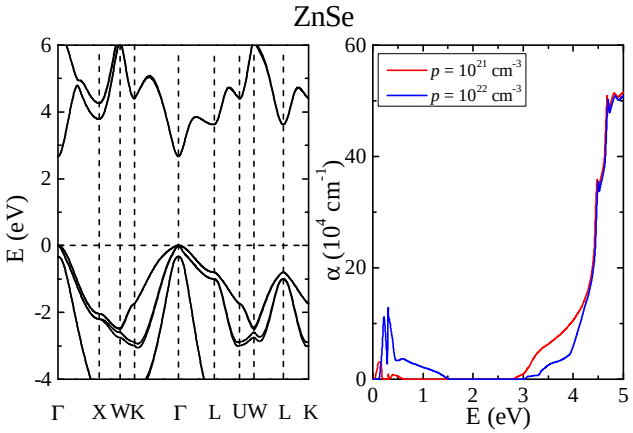

Figure S19: The band structure and absorption spectrum of ZnSe. The valence band maximum is set to energy zero.