Electronic Supplementary Information

"Structural and Chemical Features Giving Rise to Defect Tolerance of Binary Semiconductors"

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GW Band Edge Shifts

Table S1: Valence (ΔE_{VBM}) and conduction (ΔE_{CBM}) band edge shifts (in eV) calculated with GW. Band edge shifts due to spin-orbit coupling (calculated with DFT-PBE) are also included. The band edge shifts are relative to the DFT-PBE Kohn-Sham energies corresponding to the band edges.

Compound	Space Group	ΔE_{VBM} (eV)	ΔE_{CBM} (eV)
InI	63	-0.414	0.313
TlI	63	-0.458	0.287
SnI_2	14	-0.293	0.295
PbI_2	164	-0.423	0.354
SbI_3	148	-0.010	0.358
BiI_3	148	-0.104	-0.468
TlBr	221	-1.204	-0.094
TlI	221	-0.819	-0.445
InI	221	-0.575	0.224
PbI_2	224	-0.251	0.559
WO_3	14	-0.366	1.003

Comparison of Calculated and Measured Band Gaps

Table S2: Calculated (GW method) band gaps (in eV) are in good agreement with measured band gaps.

Compound	Space Group	$E_{g,GW}$	$E_{g,expt}$
InI	63	2.0	2.0[1]
TlI	63	2.9	2.9[2]
SbI_3	148	2.5	2.3[3]
BiI_3	148	2.1	2.0[4]
TlBr	221	3.0	2.7[5]
TlI	221	2.1	1.9[5]

Dielectric Constants

Table S3: Calculated dielectric constants, including electronic and ionic contributions.

Compound	Space Group	Dielectric Constant
InI	63	42
TlI	63	30
SnI_2	14	44
PbI_2	164	17
SbI_3	148	15
BiI_3	148	11
TlBr	221	79
TlI	221	90
InI	221	8
PbI_2	224	12
WO_3	14	14

Defect Formation Energies: Cubic TlBr (CsCl Structure)

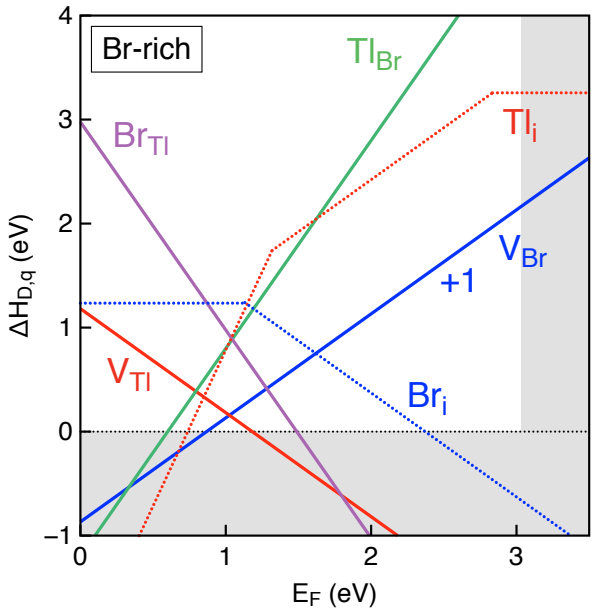

Figure S1: Defect energetics of cation and anion vacancies, antisites, and interstitials in the CsCl structure of TlBr. Interstitial defects are not the dominant (lowest-energy) defects owing to their high formation energy at the position of the equilibrium Fermi energy.

References

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