Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Explanation of the Conductivity Difference of Half-Heusler Transparent Conductors by Ionization Energy

Mi Zhong [a], *Wei Zeng* **[, b], *Fu-Sheng Liu* [a], *Bin Tang* [c], *Qi-Jun Liu** [, a]

[a] School of Physical Science and Technology, Southwest Jiaotong University, Key Laboratory of Advanced Technologies of Materials, Ministry of Education of China, Chengdu 610031, People's Republic of China

[b] Teaching and Research Group of Chemistry, College of Medical Technology, Chengdu University of Traditional Chinese Medicine, Chengdu 610075, People's Republic of China

[c] State Key Laboratory of Solidification Processing, Northwestern Polytechnical University, Xi'an 710072, People's Republic of China.

Corresponding Author

* E-mail: qijunliu@home.swjtu.edu.cn

** E-mail: zengwei_chemistry@126.com

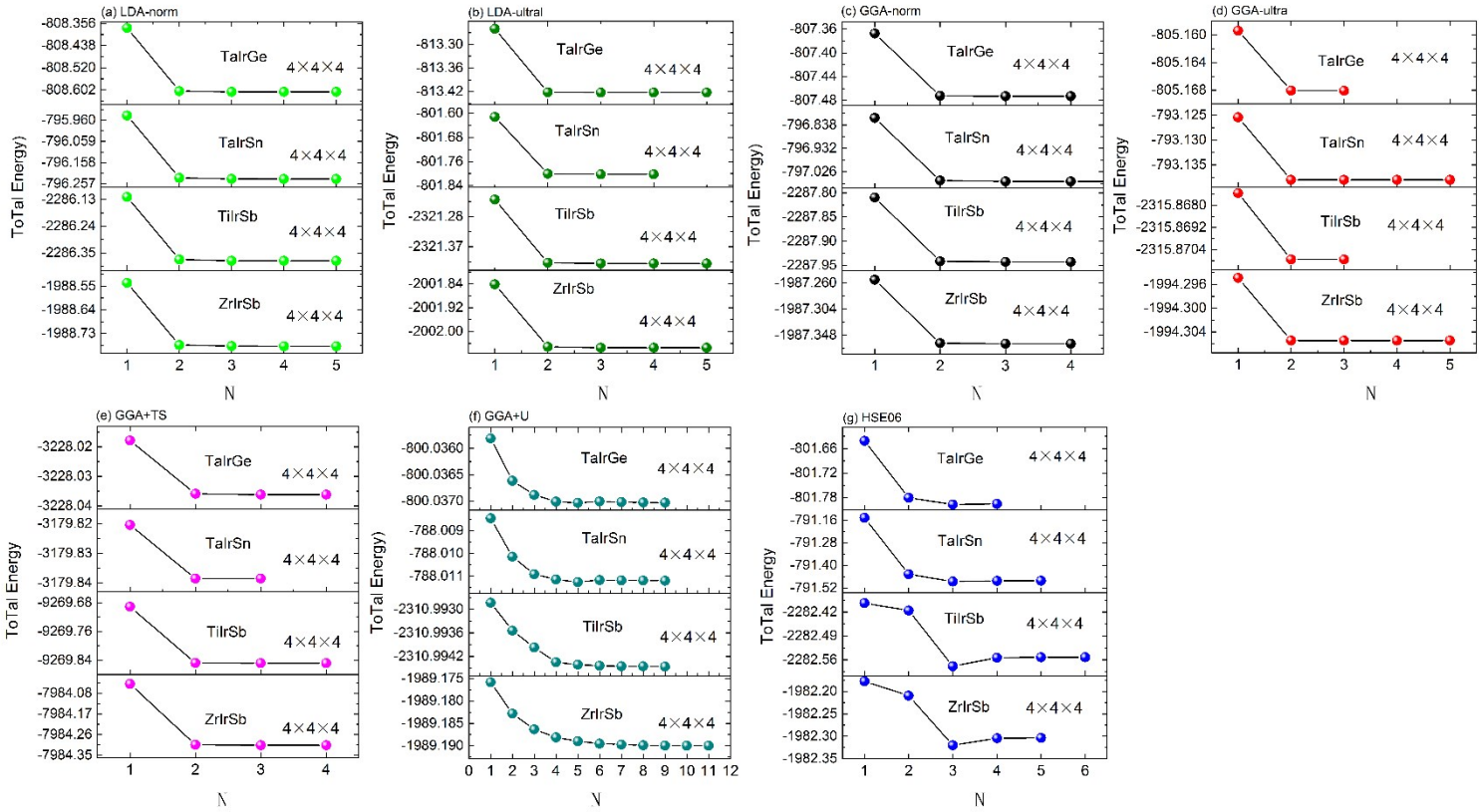

Figure S1. Calculated total energy as a function of N for ABX compounds with LDA, GGA, GGA+TS, GGA+U and HSE06 functional for testing the convergence of the k-point mesh.

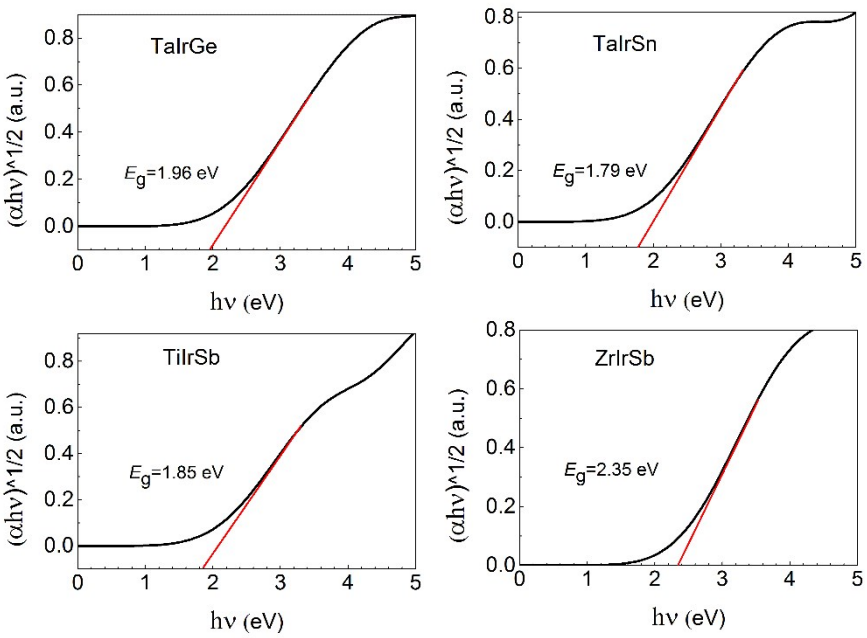

Figure S2. The determination of indirect band gaps of ABX compounds (HSE06).

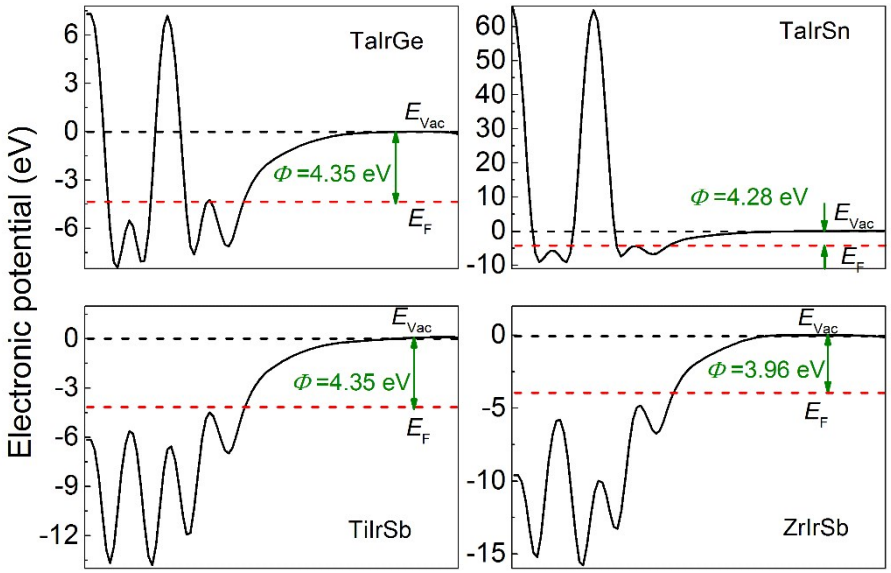

Figure S3. Calculated electrostatic potentials ABX system with slab with a width of 7 layers.

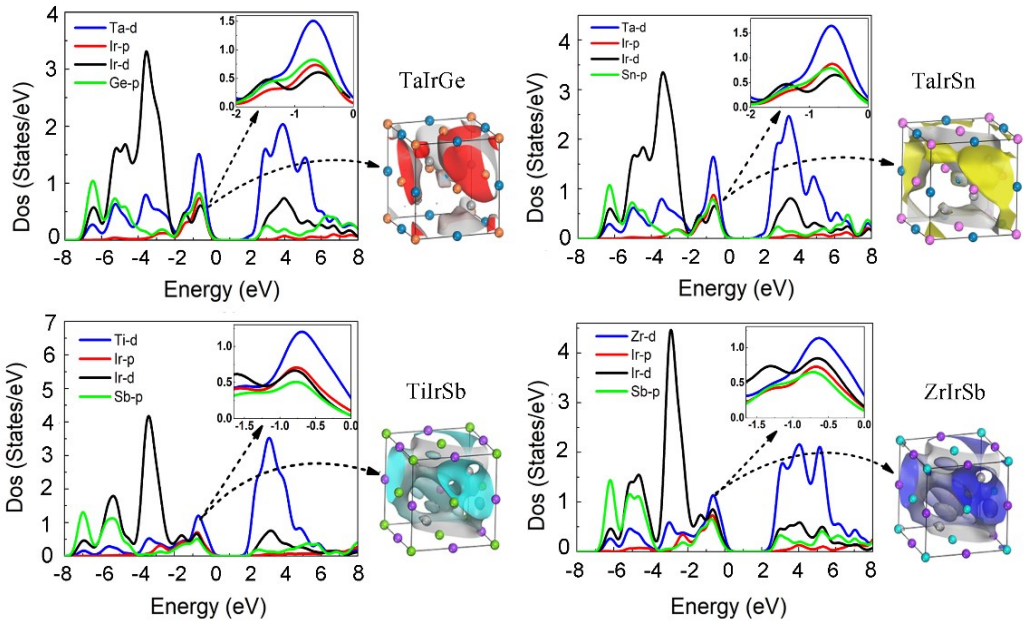

Figure S4. Partial density of states (PDOS) of TaIrGe, TaIrSn, TiIrSb, and ZrIrSb within HSE06. The corresponding modulus of the crystalline orbital near the valence band edge, and isovalue of 5×10^{-2} a.u is adopted

Table S1 The calculated lattice constants of TaIrGe, TaIrSn, TiIrSb and ZrIrSb along with the previous reported values.

	a (LDA-ultra)	*a* (LDA-norm)	*a* (GGA-ultra)	*a* (GGA-norm)	*a* (GGA+TS)	*a* (GGA+U)	*a* (HSE06)	Ref. [9]
TaIrGe	5.893	5.861	6.059	5.914	6.002	6.039	5.852	6.026
	-2.21%	-2.74%	0.55%	-1.86%	-0.40%	0.22%	-2.89%	
TaIrSn	6.085	6.043	6.273	6.054	6.206	6.253	5.997	6.233
	-2.37%	-3.05%	0.64%	-2.87%	-0.43%	0.32%	-3.79%	
TiIrSb	6.010	5.980	6.148	6.032	6.093	6.159	5.881	6.169
	-2.58%	-3.06%	-0.34%	-2.22%	-1.23%	-0.16%	-4.67%	
ZrIrSb	6.200	6.189	6.334	6.246	6.275	6.327	6.106	6.372
	-2.70%	-2.87%	-0.60%	-1.98%	-1.52%	-0.71%	-4.17%	

Table S2 The calculated band gaps using different functional along with the previously experimental and theoretical results.

$E_{g(}E_{g}^{dir})$	GGA	GGA+TS	GGA+U	HSE06	Exp.[9, 18]	HSE06 [9]	HSE06[18]
TaIrGe	1.20	1.19	1.62 (2.68)	1.84 (3.19)	3.36 [18]	1.62 (2.49)	1.74 (3.1)
TaIrSn	1.16	1.16	1.54 (2.24)	1.75 (2.77)	2.4 [9]	1.55 (2.26)	1.61 (2.33)
TiIrSb	0.98	1.01	1.41 (2.16)	1.81 (2.64)	2.4 [9]	1.63 (2.39)	1.69 (2.51)
ZrIrSb	1.61	1.65	1.82 (2.43)	2.22 (3.12)	3.2 [9]	1.91 (2.25)	2.06 (2.38)

Table S3. The effective masses of holes at VBM, Sub-VBM (sub-maximum of valence bands), and CBM.

System	VBM-L	VBM-R	Sub-VBM-L	Sub-VBM-R	CBM-L	CBM-R
TaIrGe	0.78	0.83	0.41	0.92	0.51	0.36
TaIrSn	0.76	0.92	0.41	1.04	0.57	0.43
TiIrSb	2.23	0.72	5.85	1.01	0.81	0.67
ZrIrSb	2.21	0.65	2.62	0.90	0.75	0.46