

Electronic Supplementary Information

First-principles insight into photoelectronic properties of Ge-based perovskites

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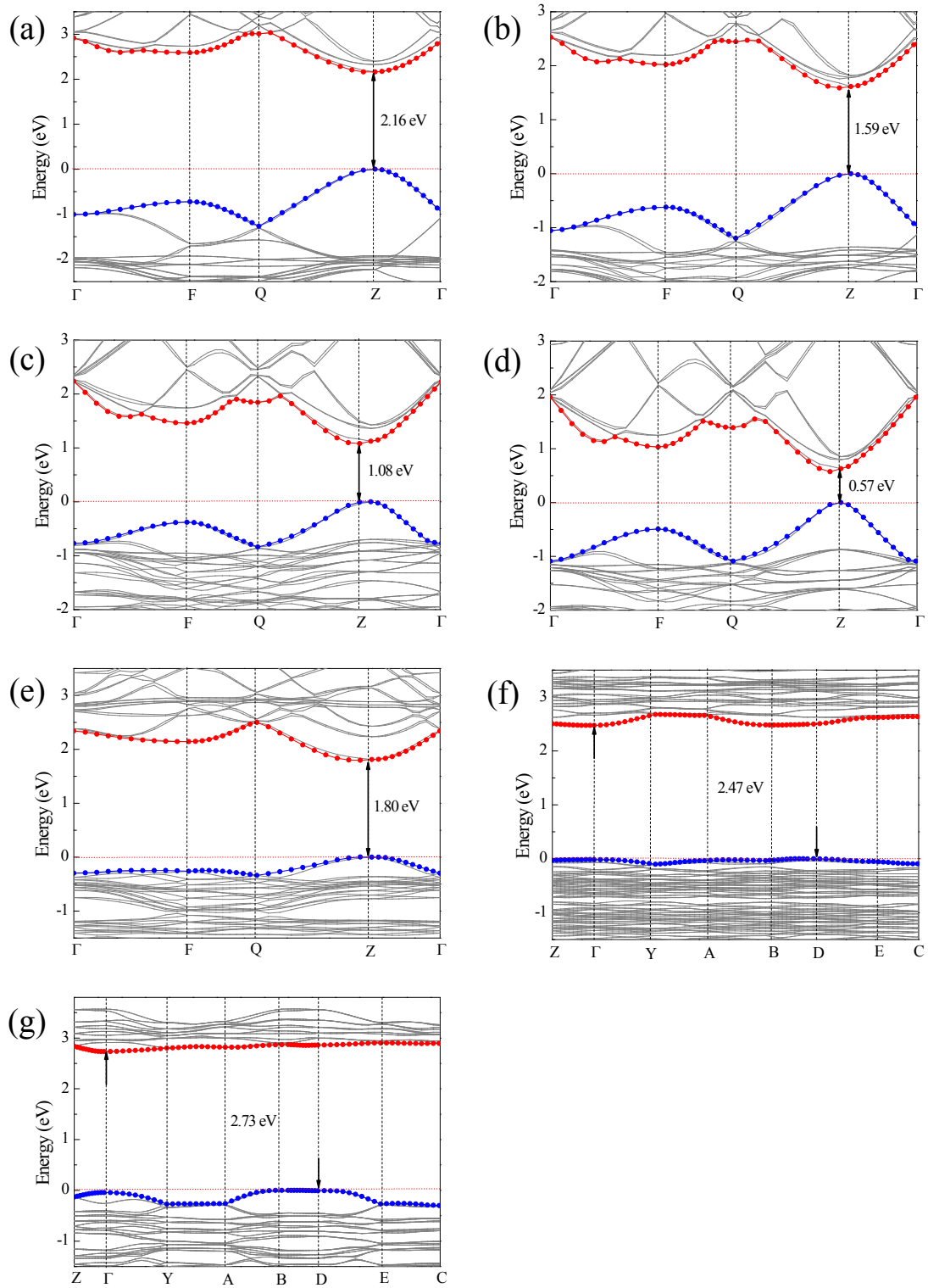


Fig. S1. The band structures of perovskites using the PBE+SOC functional: (a) MAgGeCl₃, (b) MAgGeBr₃, (c) MAgGeI₃, (d) CsGeI₃, (e) FAgGeI₃, (f) MOGeI₃, and (g) GAgGeI₃.

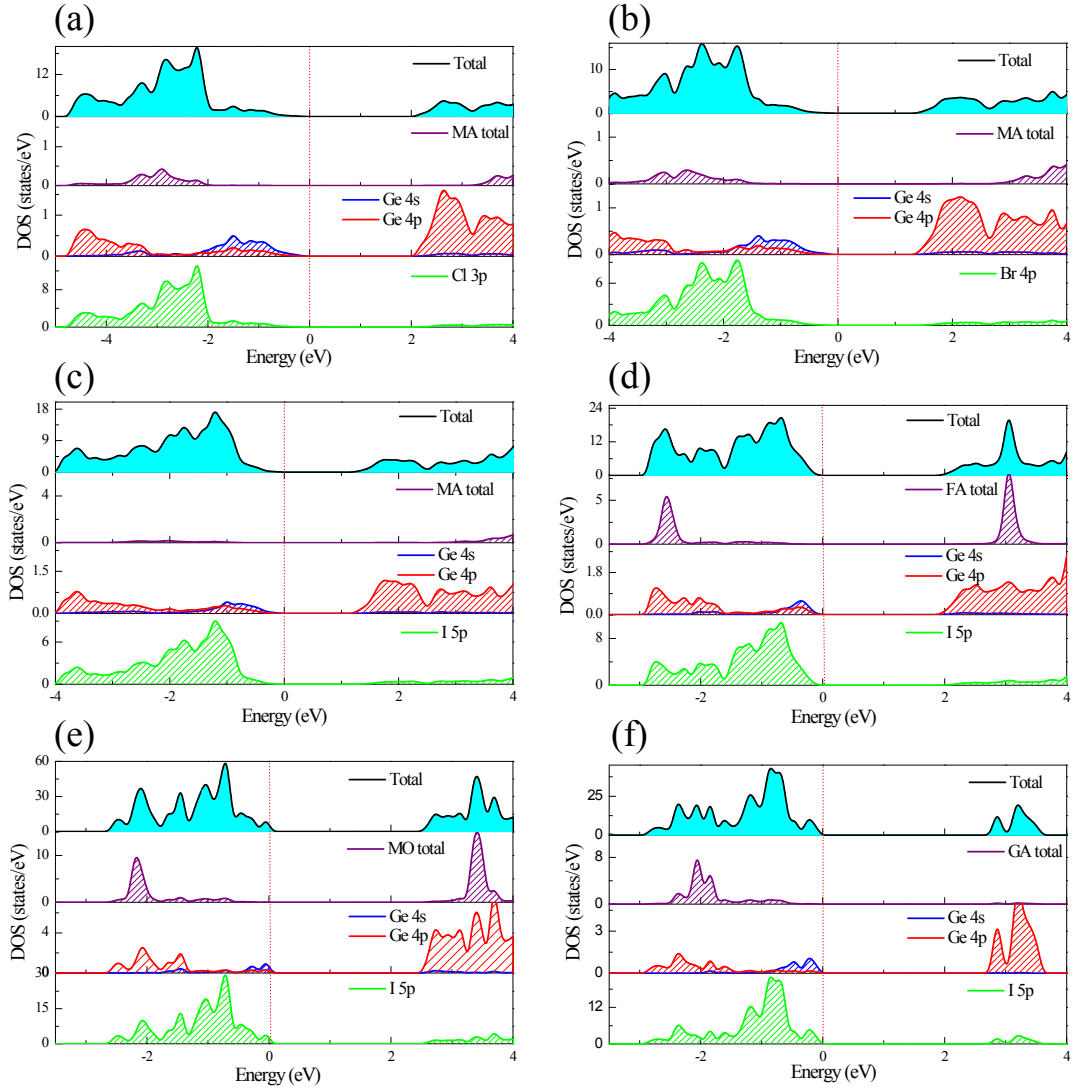


Fig. S2. The DOS of (a) MAGeCl_3 , (b) MAGeBr_3 , (c) MAGeI_3 , (d) FAGEI_3 , (e) MOGeI_3 , and (f) GAGEI_3 perovskites.

Table S1. The effective masses of electron and hole (m_e^* and m_h^* , relative to the electron static mass m_0) along the Z (0 0 0.5) \rightarrow Γ (0 0 0) direction in the trigonal perovskites by using the PBE and PBE+SOC functionals (in brackets), respectively.

Effective masses	CsGeI ₃	MAGeCl ₃	MAGeBr ₃	MAGeI ₃	FAGeI ₃
m_e^*/m_0	0.22 (0.25)	0.77 (0.73)	0.33 (0.44)	0.27 (0.28)	0.66 (0.65)
m_h^*/m_0	0.23 (0.23)	0.39 (0.45)	0.33 (0.35)	0.29 (0.30)	0.76 (0.85)