Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary File

Role of Metal and Anions in Organo-Metal Halide Perovskites $CH_3NH_3MX_3$ (M: Cu, Zn, Ga, Ge, Sn, Pb; X: Cl, Br, I) on Structural and Optoelectronic Properties for Photovoltaic Applications

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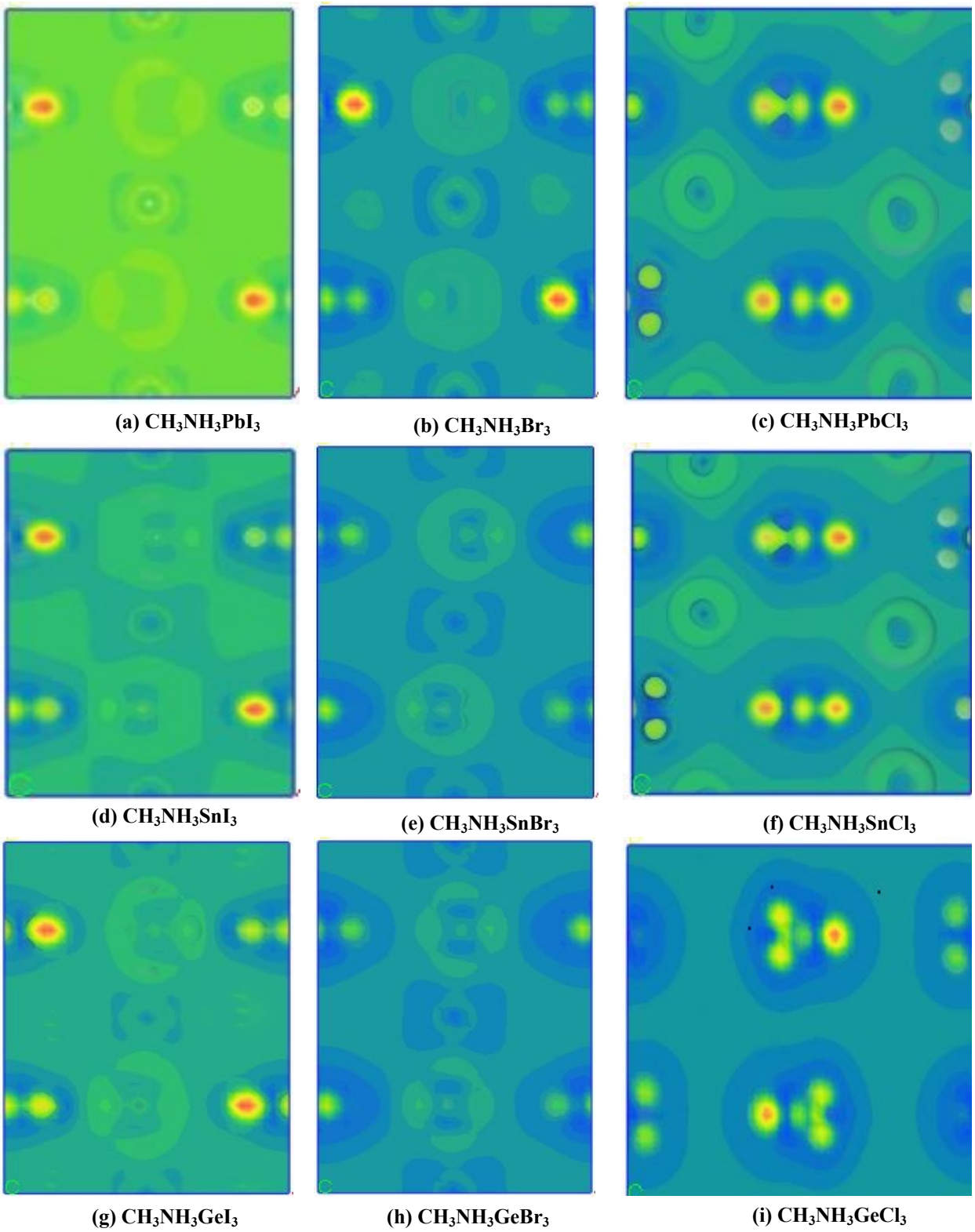
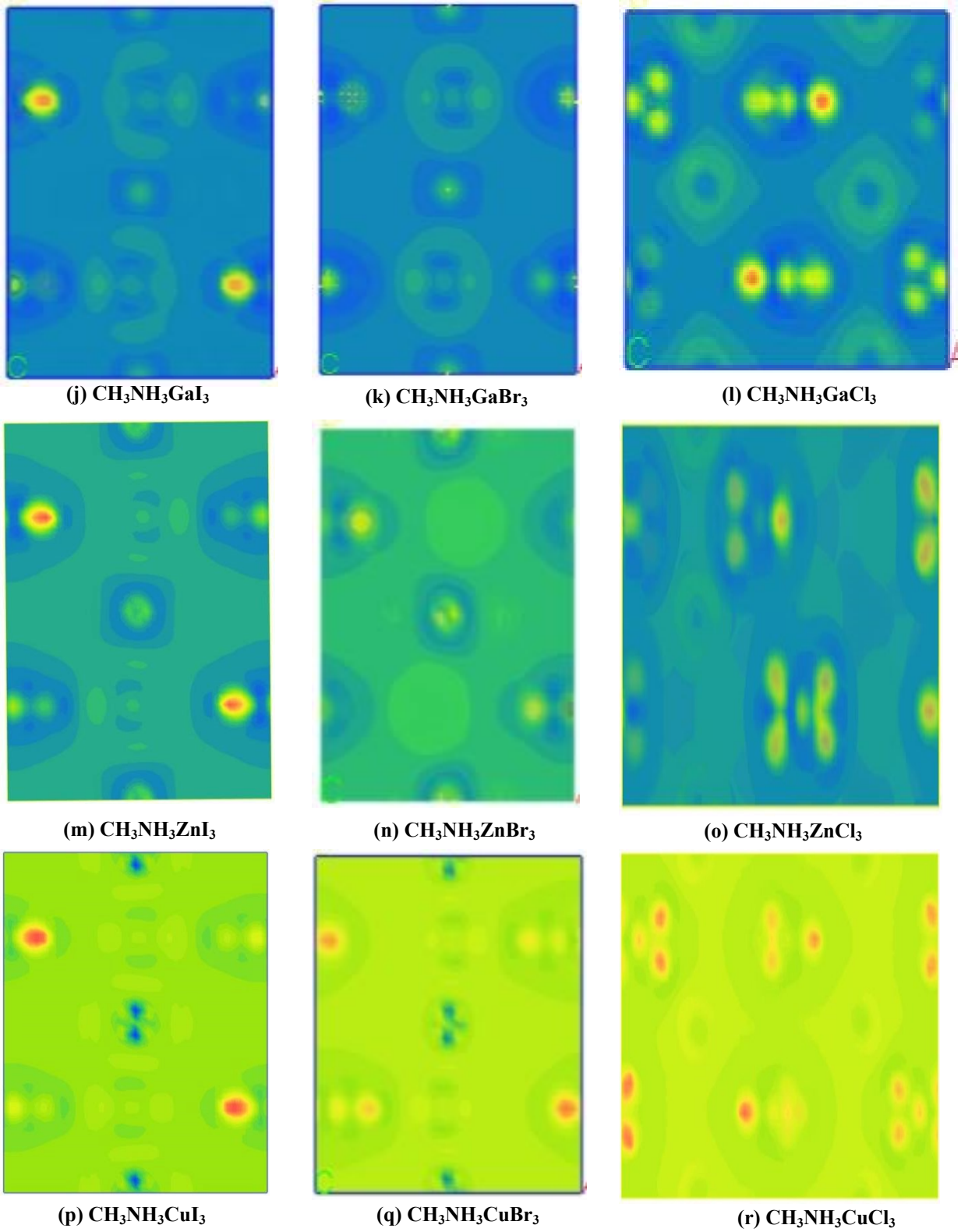


(a) $CH_3NH_3PbI_3$ (b) $CH_3NH_3Br_3$ (c) $CH_3NH_3PbCl_3$

(d) $CH_3NH_3SnI_3$ (e) $CH_3NH_3SnBr_3$ (f) $CH_3NH_3SnCl_3$

(g) $CH_3NH_3GeI_3$ (h) $CH_3NH_3GeBr_3$ (i) $CH_3NH_3GeCl_3$

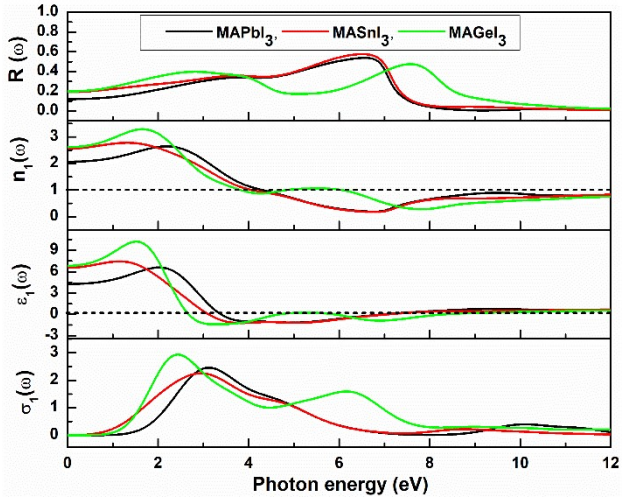


(j) $CH_3NH_3GaI_3$ (k) $CH_3NH_3GaBr_3$ (l) $CH_3NH_3GaCl_3$

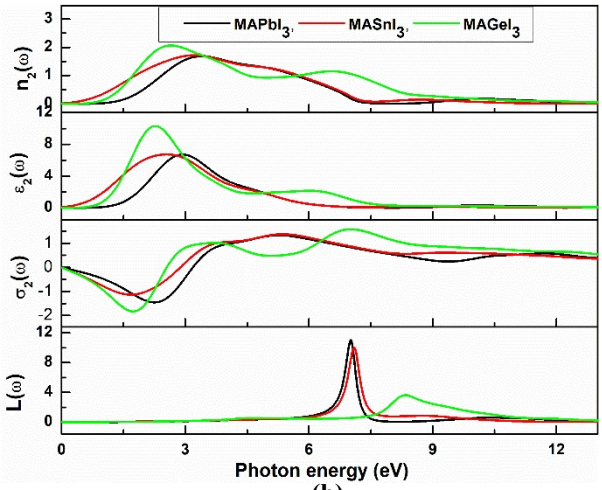
(m) $CH_3NH_3ZnI_3$ (n) $CH_3NH_3ZnBr_3$ (o) $CH_3NH_3ZnCl_3$

(p) $CH_3NH_3CuI_3$ (q) $CH_3NH_3CuBr_3$ (r) $CH_3NH_3CuCl_3$

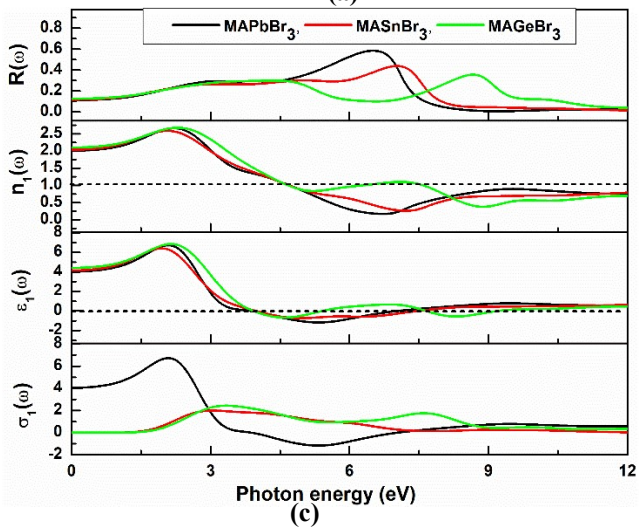
Fig. S1. Total electronic charge density for methylammonium metal halide; a field representation. The units are electrons $Å^{-3}$. In field representation, from blue to orange color symbolize the change of electron density from low to high.


MAPbI3, MASnI3, MAGeI3
R (ω)
n1(ω)
ε1(ω)
σ1(ω)
Photon energy (eV)

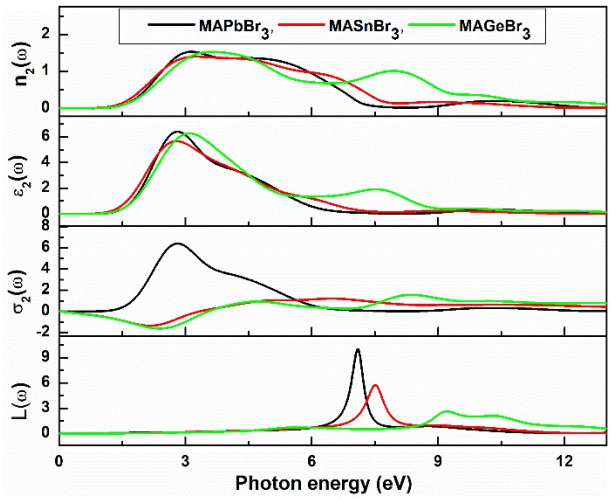
(a)


MAPbI3, MASnI3, MAGeI3
n2(ω)
ε2(ω)
σ2(ω)
L(ω)
Photon energy (eV)

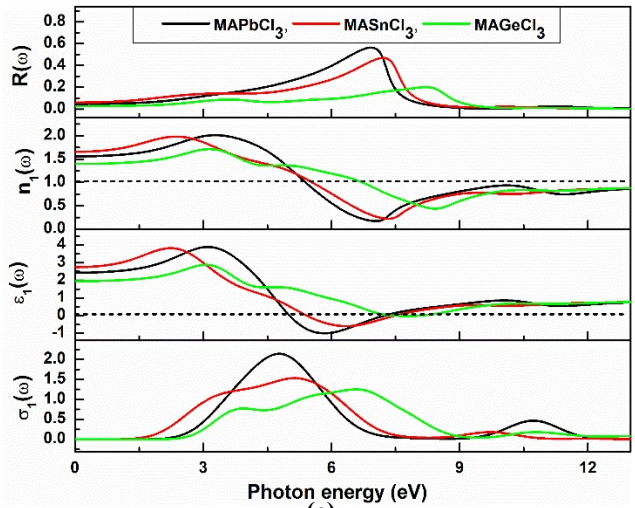
(b)


MAPbBr3, MASnBr3, MAGeBr3
R(ω)
n1(ω)
ε1(ω)
σ1(ω)
Photon energy (eV)

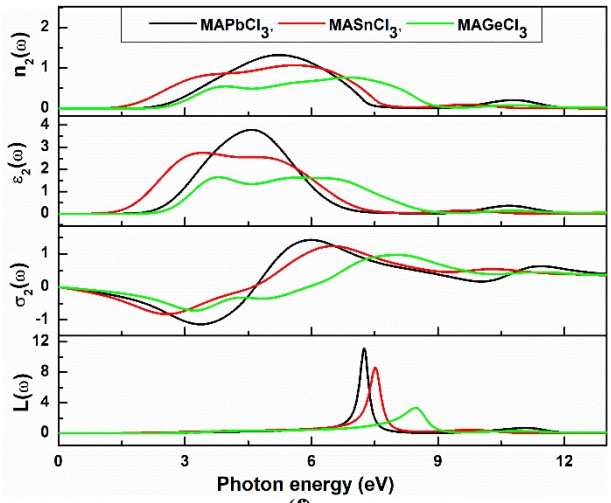
(c)


MAPbBr3, MASnBr3, MAGeBr3
n2(ω)
ε2(ω)
σ2(ω)
L(ω)
Photon energy (eV)

(d)


MAPbCl3, MASnCl3, MAGeCl3
R(ω)
n1(ω)
ε1(ω)
σ1(ω)
Photon energy (eV)

(e)


MAPbCl3, MASnCl3, MAGeCl3
n2(ω)
ε2(ω)
σ2(ω)
L(ω)
Photon energy (eV)

(f)

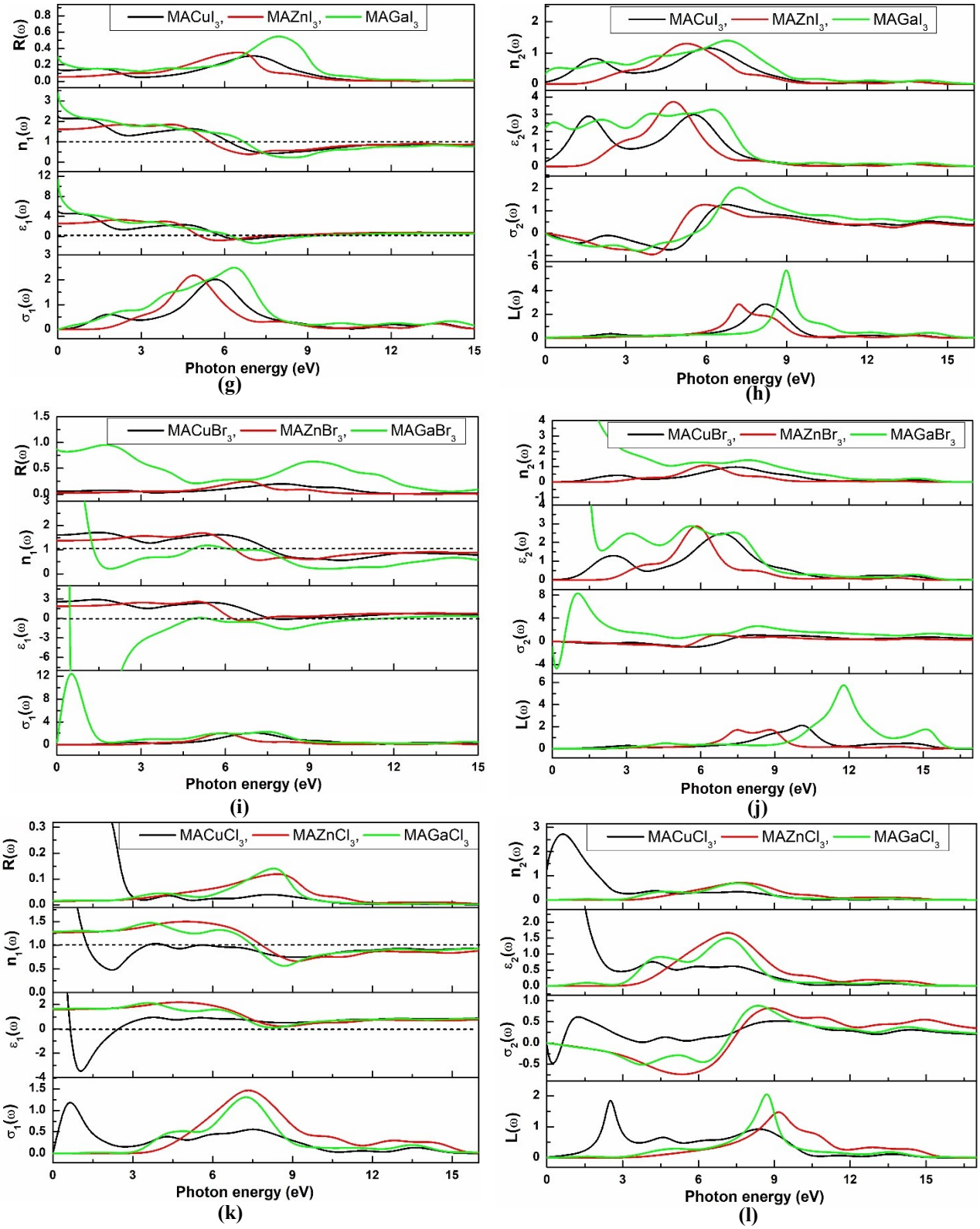


Fig. S2. Representation of different optical properties of orthorhombic $CH_3NH_3MX_3$ (where CH_3NH_3= MA, M: Cu, Zn, Ga, Ge, Sn, Pb; X: Cl, Br, I). Reflectivity R(ω), Real part of the refractive index $n_1(\omega)$, dielectric constant $\varepsilon_1(\omega)$, and optical conductivity $\sigma_1(\omega)$ as a function of energy in eV are illustrated in (a), (c), (e), (g), (i) and (K); Imaginary

part of the refractive index $n_2(\omega)$, dielectric constant $\varepsilon_2(\omega)$, and optical conductivity $\sigma_2(\omega)$ and energy loss function $L(\omega)$ are shown in (b), (d), (f), (h), (j) and (l).