First-principles calculations of optical constants

This file shows figures of optical constants for 35 semiconductors in the loss energy range 0.1 eV to 1.0 MeV.

The calculation methods are described in Ref.[1]:

The imaginary part ε_2 of the dielectric function is calculated from the WIEN2k [2] and FEFF [3] codes. WIEN2k is used to calculate the electronic state of valence electrons and to calculate lower energy losses, from 0.1 to 100 eV. FEFF deals with photoionization of inner-shell electrons and is used to calculate higher energy losses, from 10 eV to 1 MeV. We can get ε_2 over a wide loss energy range (0.1 eV – 1 MeV) by connecting its values at around 50 eV. Then, we calculate the real part of the dielectric function, ε_1, using the Kramers–Kronig relation. Using ε_1 and ε_2, we finally obtain the refractive index n, the extinction coefficient k, and the energy loss function, ELF.

Contents:

List of materials:

AgBr, AgCl, AgI, AlAs, AlN, AlSb,
c-BN, h-BN, CdS, c-CdSe, h-CdSe, CdTe,
C(diamond), GaAs, GaN, GaP, GaSb, GaSe,
Ge, InAs, InP, InSb, PbS, PbSe,
PbTe, Se, Si, c-SiC, h-SiC, SnTe,
Te, c-ZnS, h-ZnS, ZnSe, ZnTe

Note:

In each figure in Pages 2-11, the curve for each material is plotted by shifting parallel to the y-axis in order to avoid overlapping. For example, "AlSb (+10)" means that the original value was added by 10, and "AlSb (x10^5)" means that the original value was multiplied by 10^5.

References:

[1] Hiroshi Shinotsuka, Hideki Yoshikawa, Shigeo Tanuma, First-principles calculations of optical energy loss functions for 30 compound and 5 elemental semiconductors. Submitted to e-Journal of Surface Science and Nanotechnology.

[2] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, and J. Luitz, WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Tech. Universität Wien, Austria, 2001). ISBN 3-9501031-1-2.

[3] A. L. Ankudinov, C. Bouldin, J. J. Rehr, J. Sims, and H. Hung, Phys. Rev. B 65, 104107 (2002). https://doi.org/10.1103/PhysRevB.65.104107.

Energy loss function in linear scale

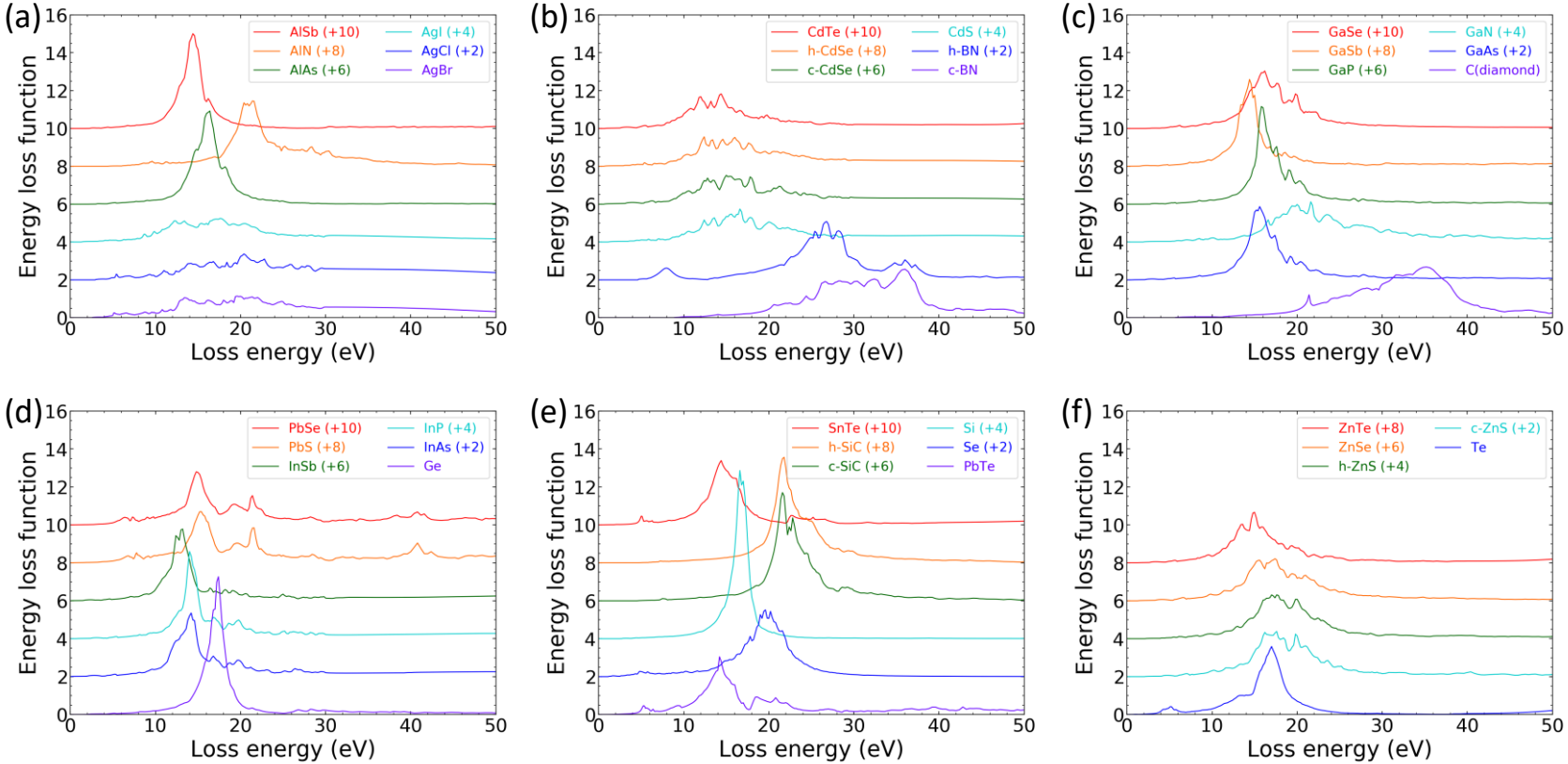

Figure 1. Plots of Energy loss function as a function of loss energy in linear scale for
(a) AgBr, AgCl, AgI, AlAs, AlN and AlSb, (b) c-BN, h-BN, CdS, c-CdSe, h-CdSe and CdTe, (c) C(diamond), GaAs, GaN, GaP, GaSb and GaSe,
(d) Ge, InAs, InP, InSb, PbS and PbSe, (e) PbTe, Se, Si, c-SiC, h-SiC and SnTe, and (f) Te, c-ZnS, h-ZnS, ZnSe and ZnTe.

Energy loss function in log scale

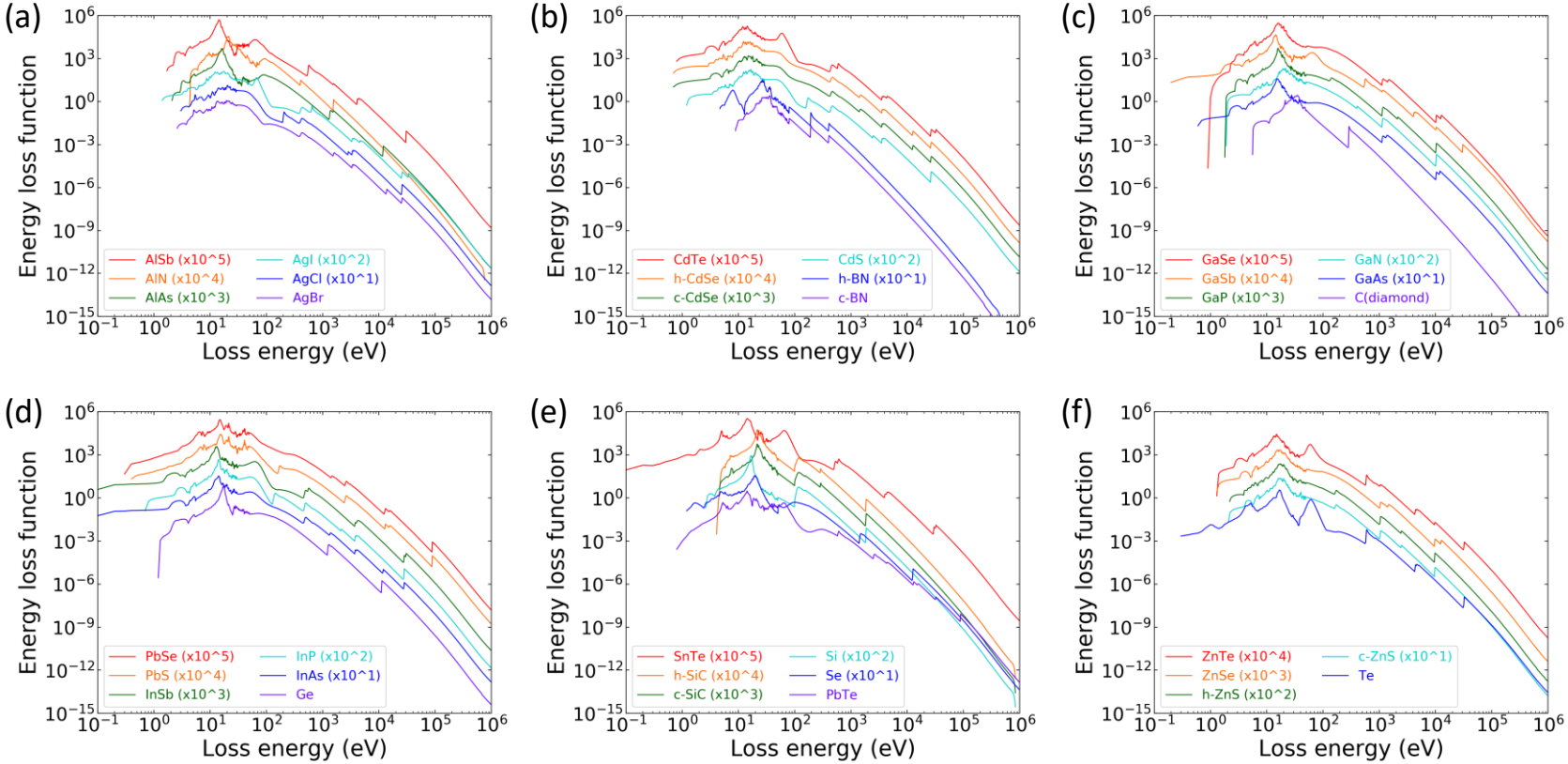

Figure 2. Plots of Energy loss function as a function of loss energy in log scale for
(a) AgBr, AgCl, AgI, AlAs, AlN and AlSb, (b) c-BN, h-BN, CdS, c-CdSe, h-CdSe and CdTe, (c) C(diamond), GaAs, GaN, GaP, GaSb and GaSe,
(d) Ge, InAs, InP, InSb, PbS and PbSe, (e) PbTe, Se, Si, c-SiC, h-SiC and SnTe, and (f) Te, c-ZnS, h-ZnS, ZnSe and ZnTe.

Refractive index in linear scale

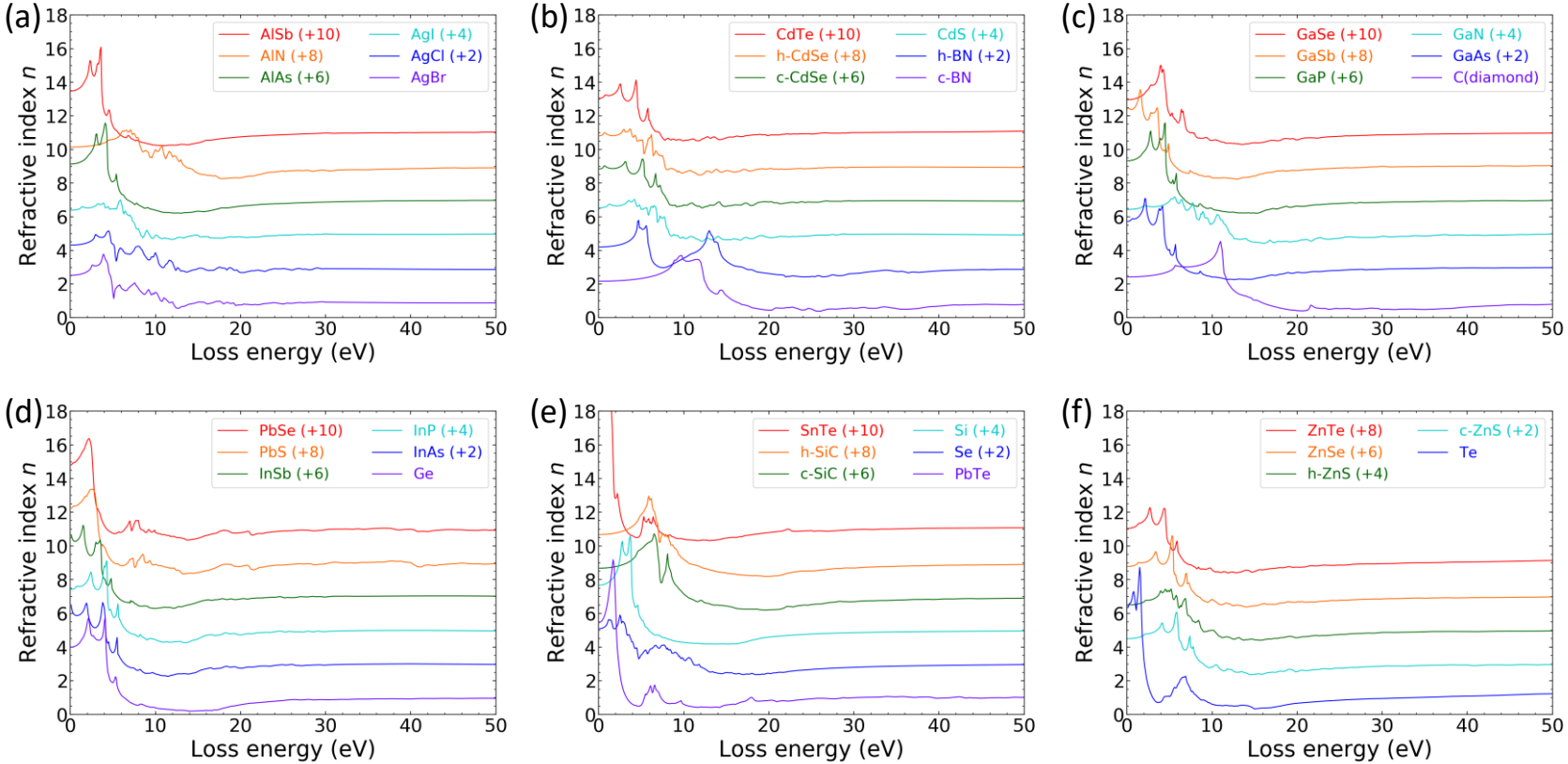

Figure 3. Plots of Refractive index as a function of loss energy in linear scale for
(a) AgBr, AgCl, AgI, AlAs, AlN and AlSb, (b) c-BN, h-BN, CdS, c-CdSe, h-CdSe and CdTe, (c) C(diamond), GaAs, GaN, GaP, GaSb and GaSe,
(d) Ge, InAs, InP, InSb, PbS and PbSe, (e) PbTe, Se, Si, c-SiC, h-SiC and SnTe, and (f) Te, c-ZnS, h-ZnS, ZnSe and ZnTe.

Refractive index in log scale

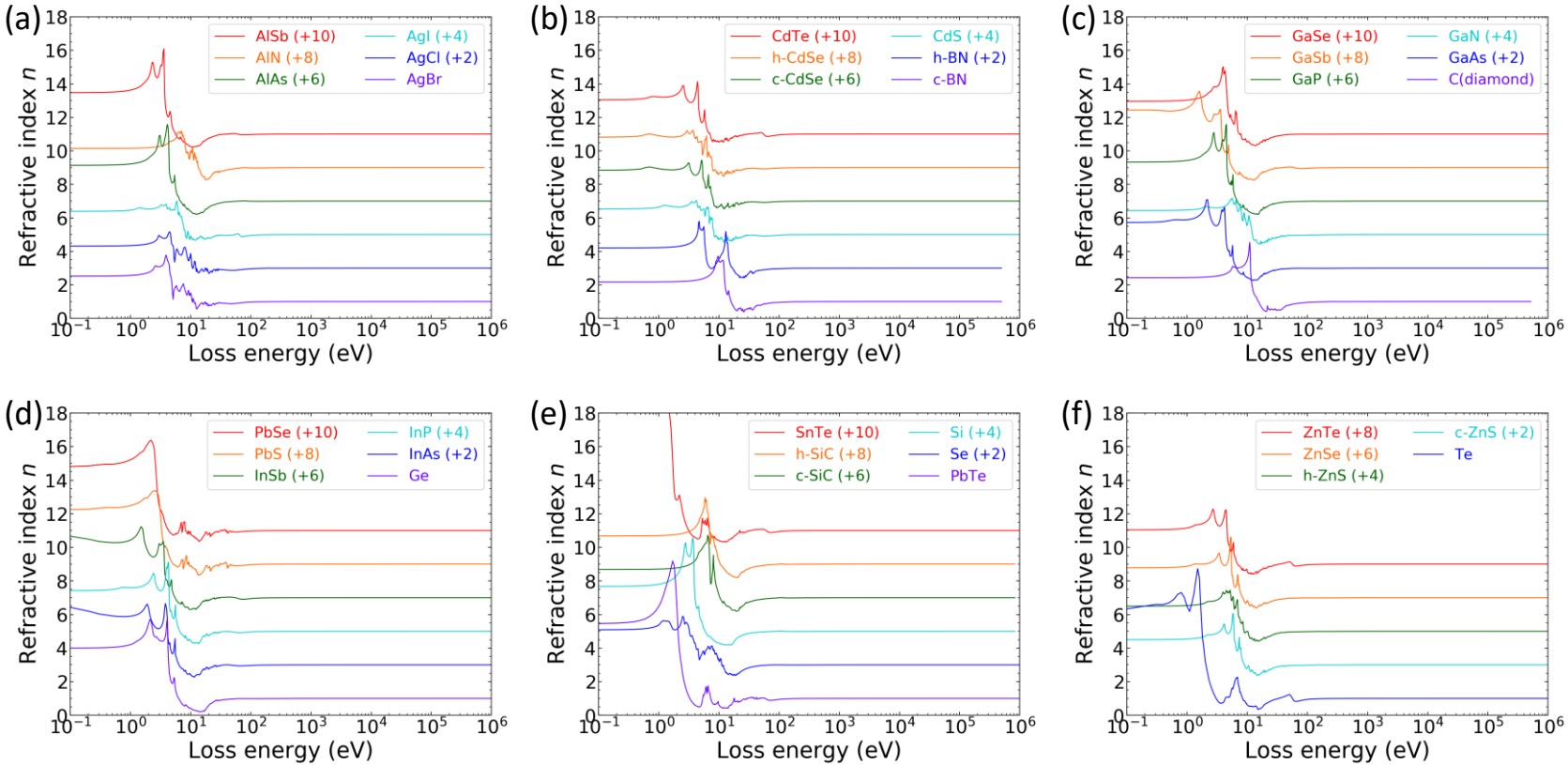

Figure 4. Plots of Refractive index as a function of loss energy in log scale for
(a) AgBr, AgCl, AgI, AlAs, AlN and AlSb, (b) c-BN, h-BN, CdS, c-CdSe, h-CdSe and CdTe, (c) C(diamond), GaAs, GaN, GaP, GaSb and GaSe,
(d) Ge, InAs, InP, InSb, PbS and PbSe, (e) PbTe, Se, Si, c-SiC, h-SiC and SnTe, and (f) Te, c-ZnS, h-ZnS, ZnSe and ZnTe.

Extinction coefficient in linear scale

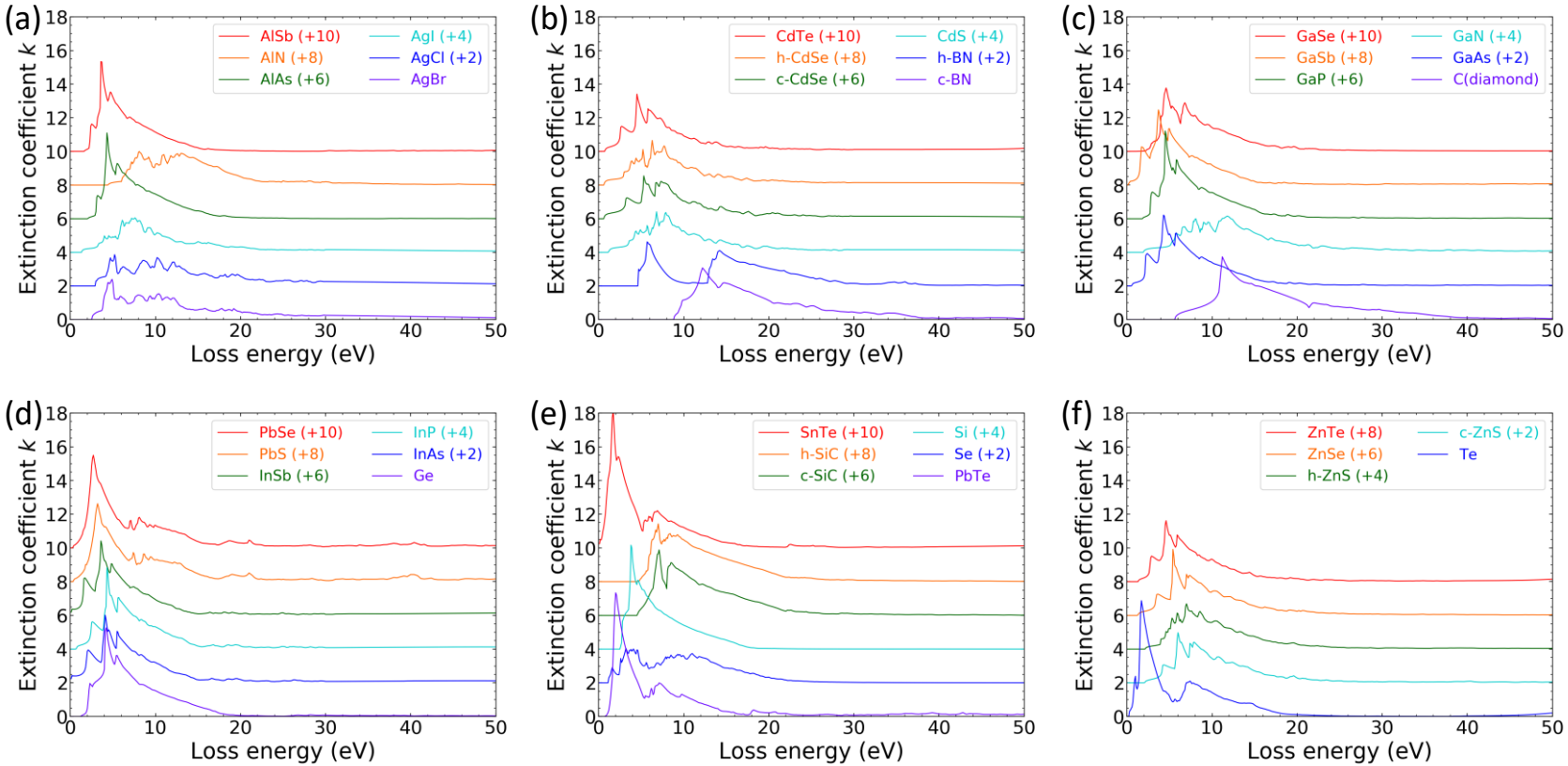

Figure 5. Plots of Extinction coefficient as a function of loss energy in linear scale for
(a) AgBr, AgCl, AgI, AlAs, AlN and AlSb, (b) c-BN, h-BN, CdS, c-CdSe, h-CdSe and CdTe, (c) C(diamond), GaAs, GaN, GaP, GaSb and GaSe,
(d) Ge, InAs, InP, InSb, PbS and PbSe, (e) PbTe, Se, Si, c-SiC, h-SiC and SnTe, and (f) Te, c-ZnS, h-ZnS, ZnSe and ZnTe.

Extinction coefficient in log scale

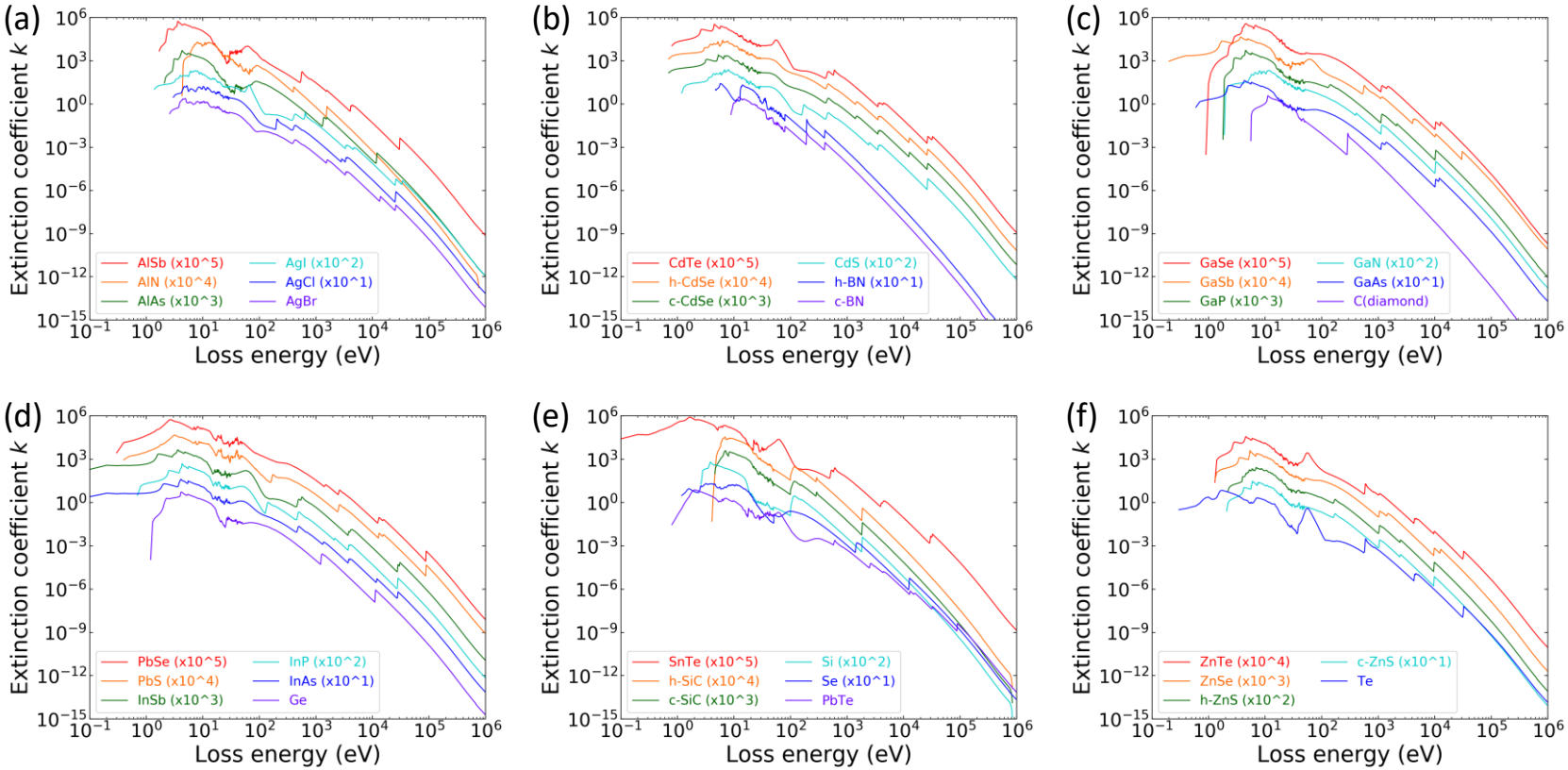

Figure 6. Plots of Extinction coefficient as a function of loss energy in log scale for
(a) AgBr, AgCl, AgI, AlAs, AlN and AlSb, (b) c-BN, h-BN, CdS, c-CdSe, h-CdSe and CdTe, (c) C(diamond), GaAs, GaN, GaP, GaSb and GaSe,
(d) Ge, InAs, InP, InSb, PbS and PbSe, (e) PbTe, Se, Si, c-SiC, h-SiC and SnTe, and (f) Te, c-ZnS, h-ZnS, ZnSe and ZnTe.

Real part of dielectric function in linear scale

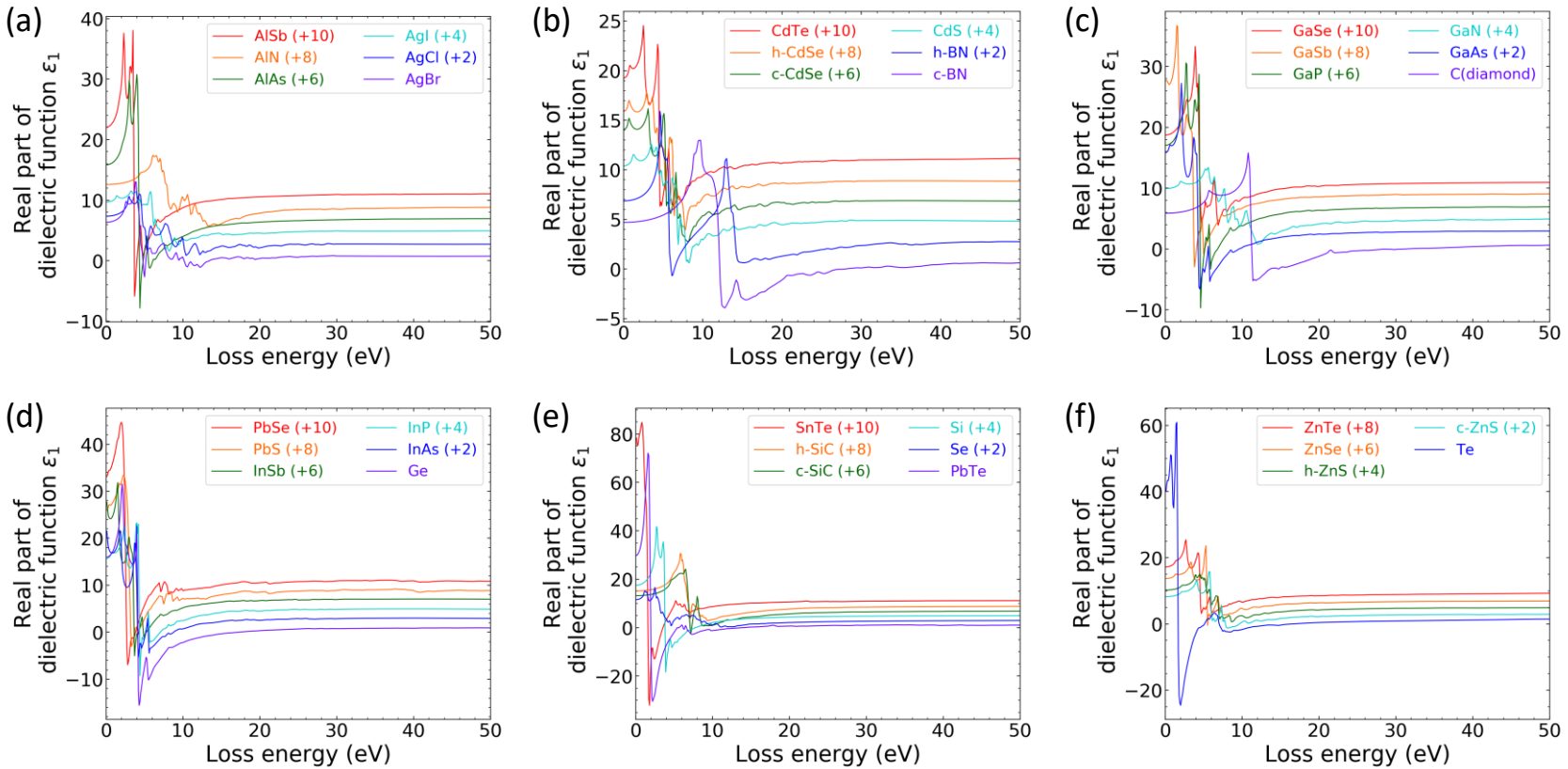

Figure 7. Plots of Real part of dielectric function as a function of loss energy in linear scale for (a) AgBr, AgCl, AgI, AlAs, AlN and AlSb, (b) c-BN, h-BN, CdS, c-CdSe, h-CdSe and CdTe, (c) C(diamond), GaAs, GaN, GaP, GaSb and GaSe, (d) Ge, InAs, InP, InSb, PbS and PbSe, (e) PbTe, Se, Si, c-SiC, h-SiC and SnTe, and (f) Te, c-ZnS, h-ZnS, ZnSe and ZnTe.

Real part of dielectric function in log scale

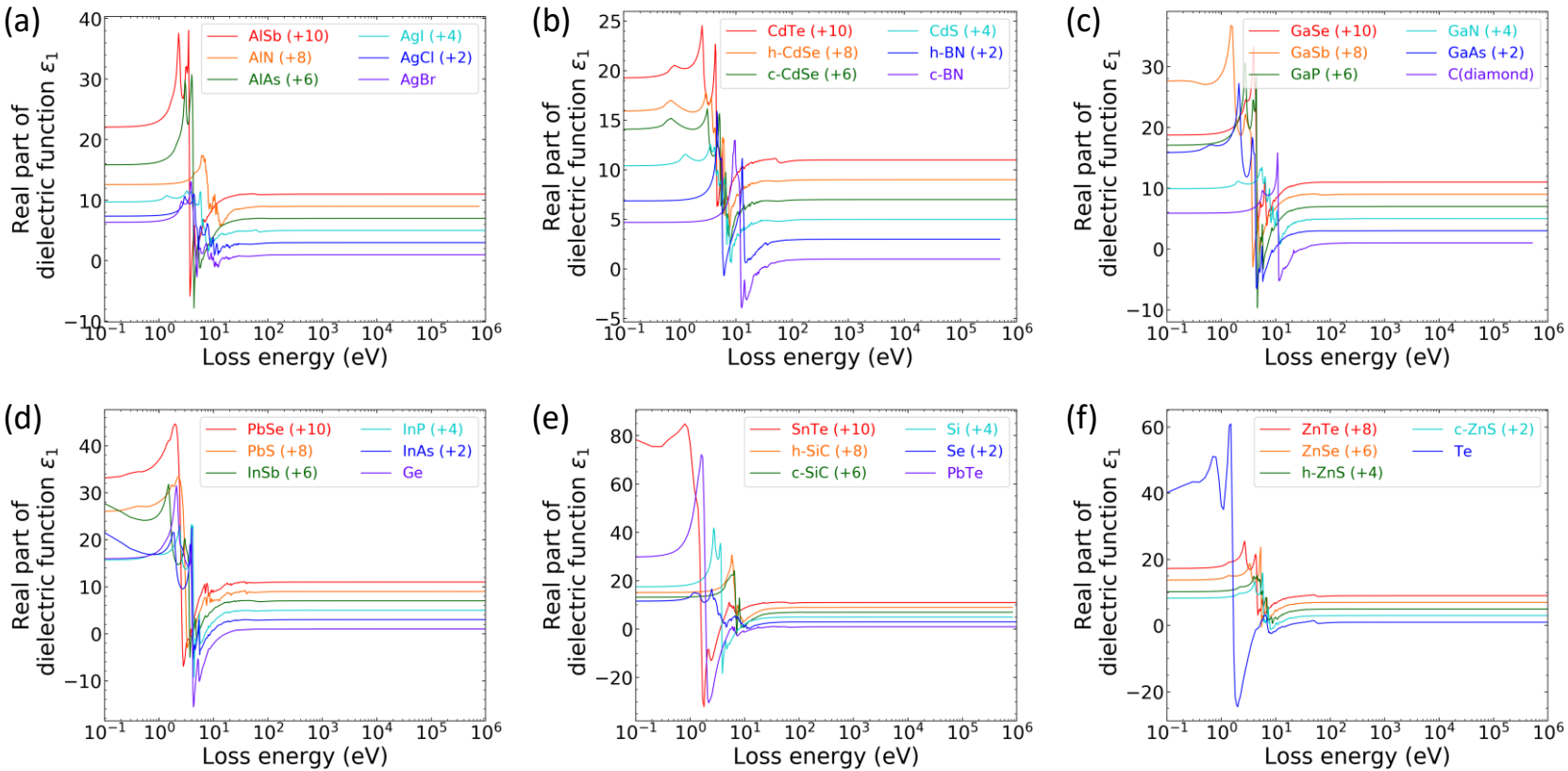

Figure 8. Plots of Real part of dielectric function as a function of loss energy in log scale for (a) AgBr, AgCl, AgI, AlAs, AlN and AlSb, (b) c-BN, h-BN, CdS, c-CdSe, h-CdSe and CdTe, (c) C(diamond), GaAs, GaN, GaP, GaSb and GaSe, (d) Ge, InAs, InP, InSb, PbS and PbSe, (e) PbTe, Se, Si, c-SiC, h-SiC and SnTe, and (f) Te, c-ZnS, h-ZnS, ZnSe and ZnTe.

Imaginary part of dielectric function in linear scale

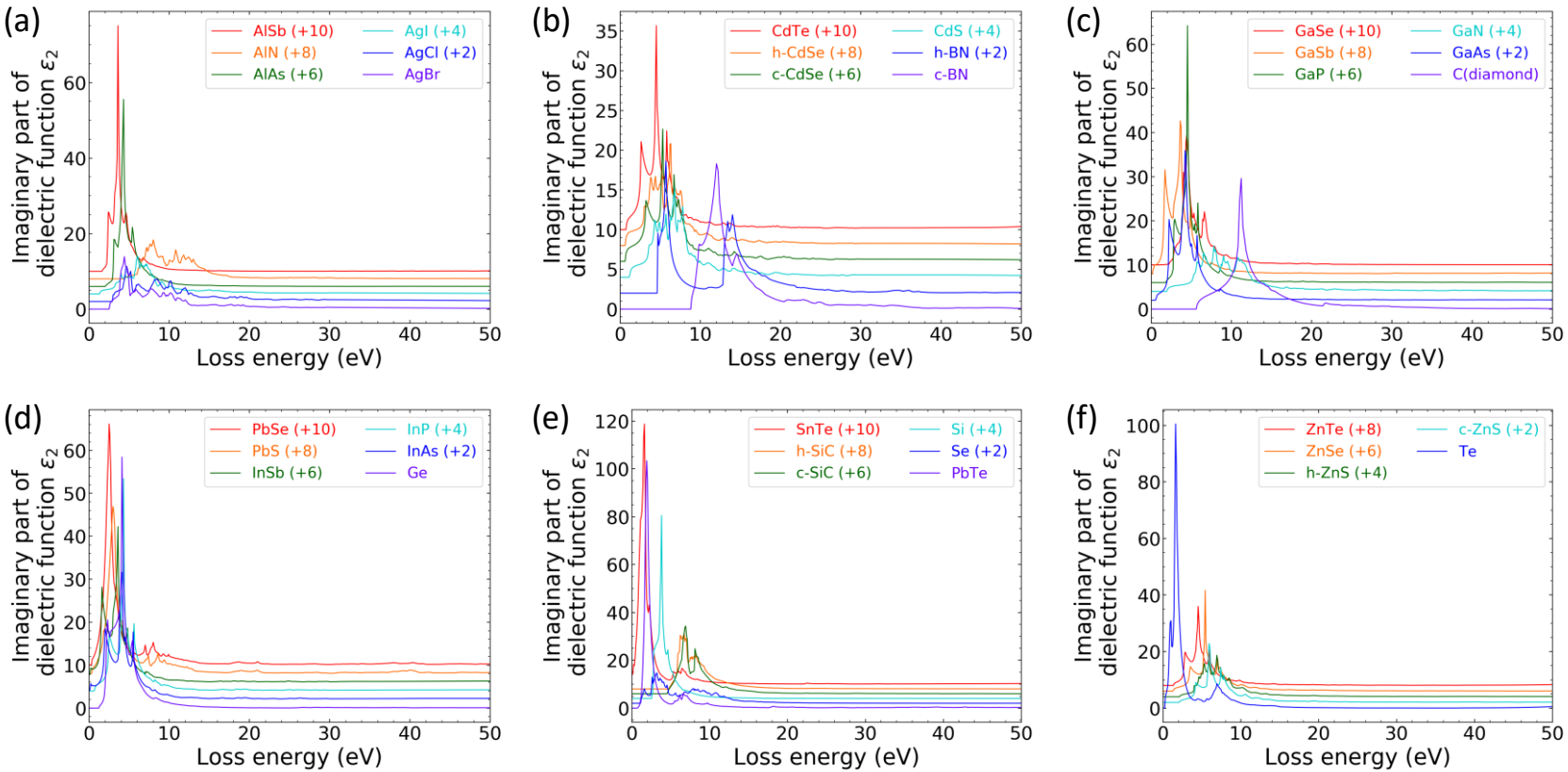

Figure 9. Plots of Imaginary part of dielectric function as a function of loss energy in linear scale for (a) AgBr, AgCl, AgI, AlAs, AlN and AlSb, (b) c-BN, h-BN, CdS, c-CdSe, h-CdSe and CdTe, (c) C(diamond), GaAs, GaN, GaP, GaSb and GaSe, (d) Ge, InAs, InP, InSb, PbS and PbSe, (e) PbTe, Se, Si, c-SiC, h-SiC and SnTe, and (f) Te, c-ZnS, h-ZnS, ZnSe and ZnTe.

Imaginary part of dielectric function in log scale

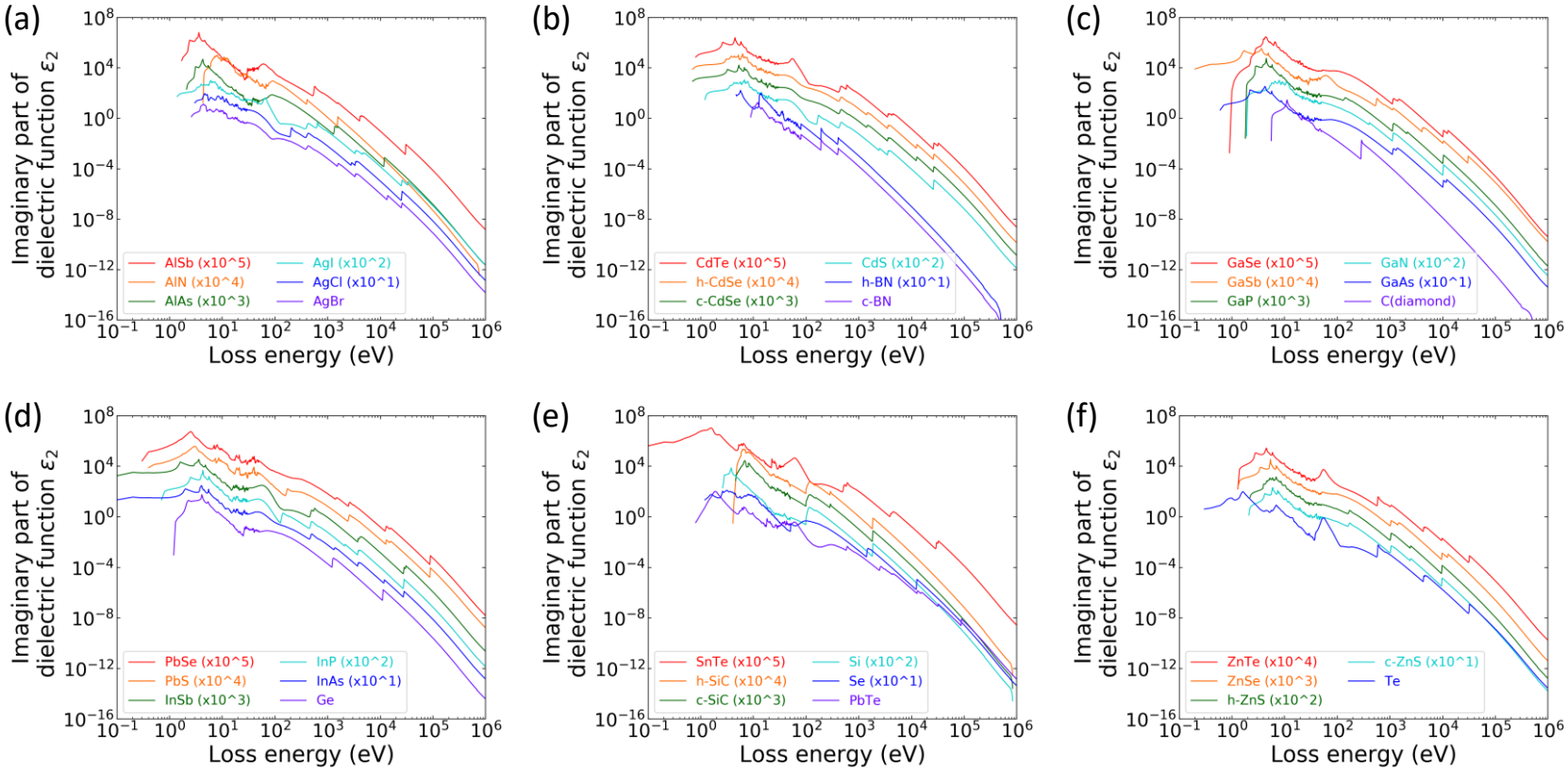

Figure 10. Plots of Imaginary part of dielectric function as a function of loss energy in log scale for (a) AgBr, AgCl, AgI, AlAs, AlN and AlSb, (b) c-BN, h-BN, CdS, c-CdSe, h-CdSe and CdTe, (c) C(diamond), GaAs, GaN, GaP, GaSb and GaSe, (d) Ge, InAs, InP, InSb, PbS and PbSe, (e) PbTe, Se, Si, c-SiC, h-SiC and SnTe, and (f) Te, c-ZnS, h-ZnS, ZnSe and ZnTe.