Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Systematic Investigation of Magneto-Electronic Structure and Optical Properties of New Halide Double Perovskites Cs_2NaMCl_6 (M=Mn, Co and Ni) by Spin Polarized Calculations

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Structural Parameters

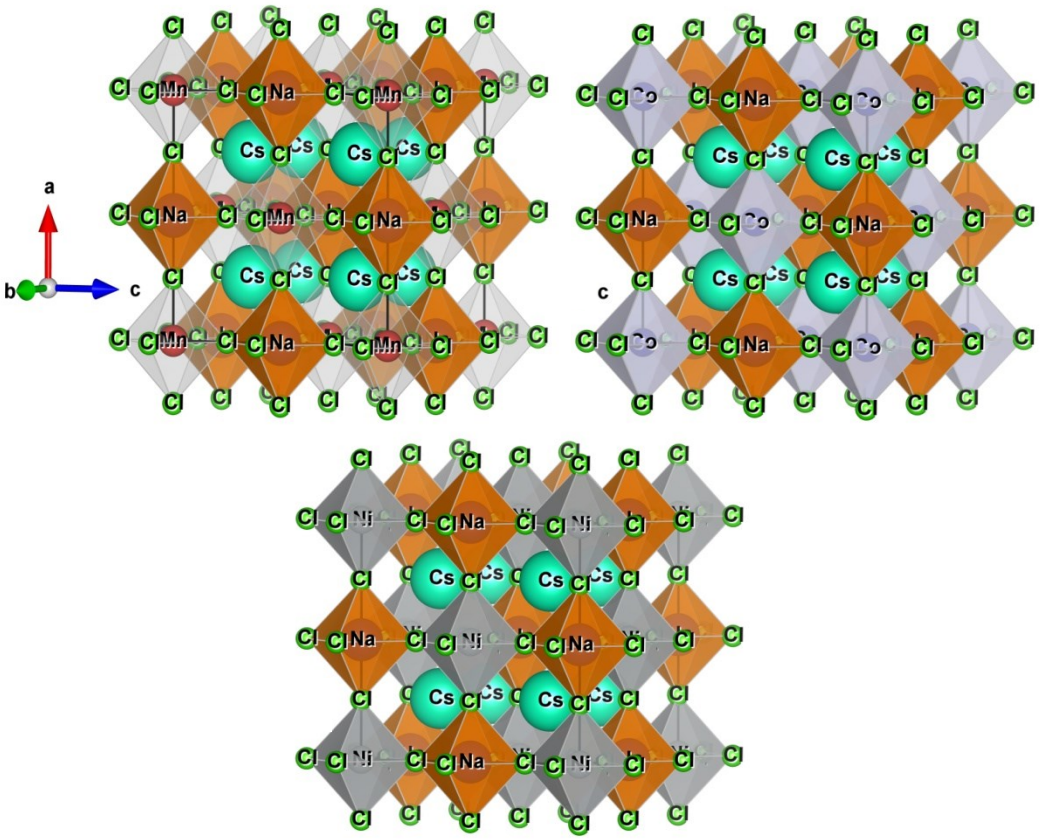

Fig. S1: Structural representation of $Cs_2NaM(Mn, Co, Ni)Cl_6$ alloys. The Na and transition atoms are engulfed by octahedra of Cl-atoms while as Cs atom is enclosed by cubo-octahedra of 12-Cl atoms

Band Structure

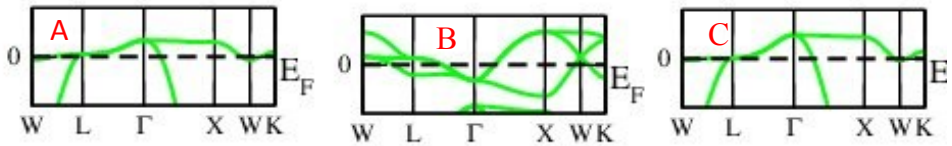

Fig. S2: Zoomed band structure in vicinity of Fermi level for (A) $Cs_2NaMnCl_6$-up; (B) $Cs_2NaCoCl_6$-dn (C) (a) $Cs_2NaNiCl_6$-up reflect the metallic nature of alloys. The crossing over of Fermi level by bands reflects the metallic character in the respective channels.

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Optical Properties

The interaction of light with matter can be revealed by analyzing the nature of the extinction coefficient k(ω) and refractive index n(ω). The variation to refractive index n(ω) with photon energy is depicted through Fig. S3(A) and the behaviour of extinction coefficients k(ω) is represented through Fig. S3(B). The variation of refractive index (n) and extinction coefficients (k) with photon energy replicates the character of real and imaginary dielectric constants, respectively.

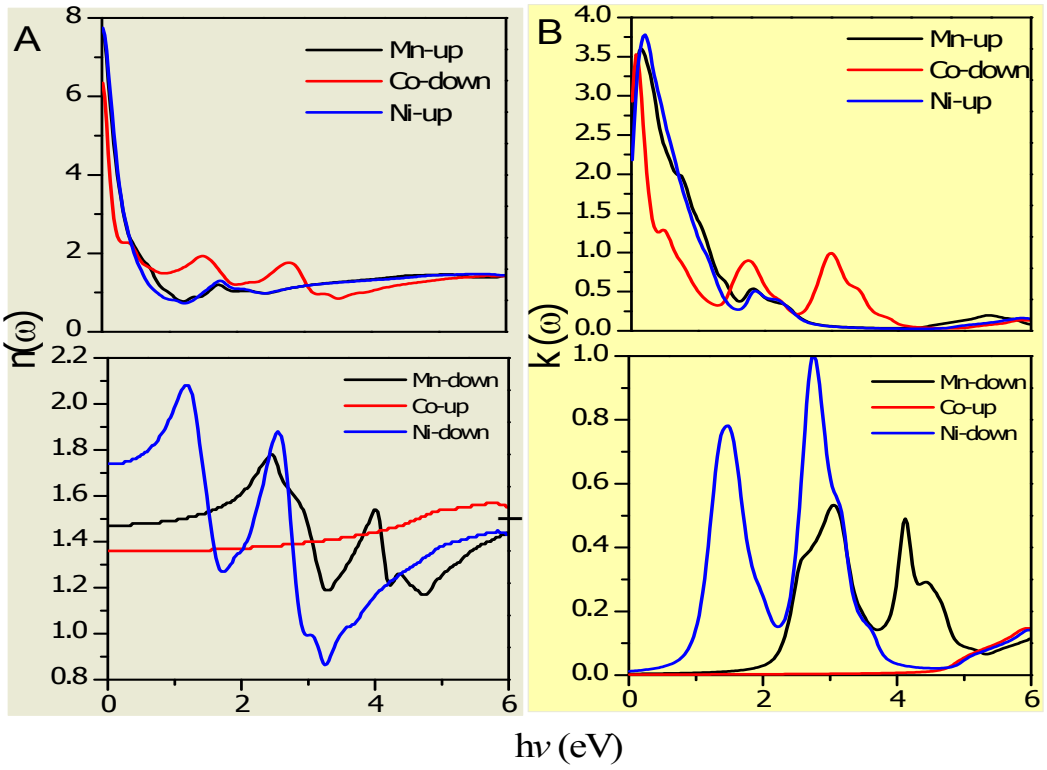

Fig. S3: Variation in reflection coefficient and extinction coefficient with photon energy (A) reflection coefficient; (B) extinction coefficient

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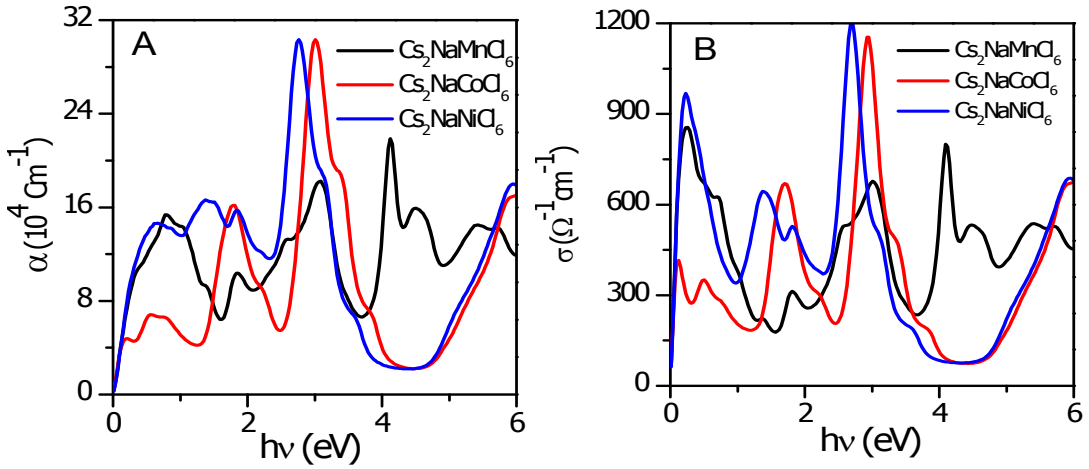

Fig. S4: (A) Total absorption power; (B) Total conductivity without considering inter-channel transitions of Cs_2NaMCl_6 double perovskites