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

Supplementary Information for:

On the Structure-Property relationships of (Al^{3+}, Ga^{3+}, In^{3+})-Doped Spinel Cobalt Ferrite Ceramics: A Combined Experimental and DFT Study

M. Naveed-Ul-Haq[1,*], Shahzad Hussain[2,*], Samira Webers[3], Soma Salamon[3], Ibtisam Ahmad[2], Tayyaba Bibi[2], Amna Hameed[2], Heiko Wende[3]

[1]Department of Physics, COMSATS University Islamabad, Lahore Campus 54000, Pakistan.
[2]Department of Physics, COMSATS University Islamabad, Pakistan.
[3]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany.
*Corresponding authors: naveedulhaq@cuilahore.edu.pk; shahzad.hussain@comsats.edu.pk

Note: This Supplementary Information contains 4 Figures (figures S-I to S-IV) and 4 Tables (table S1 to S4).

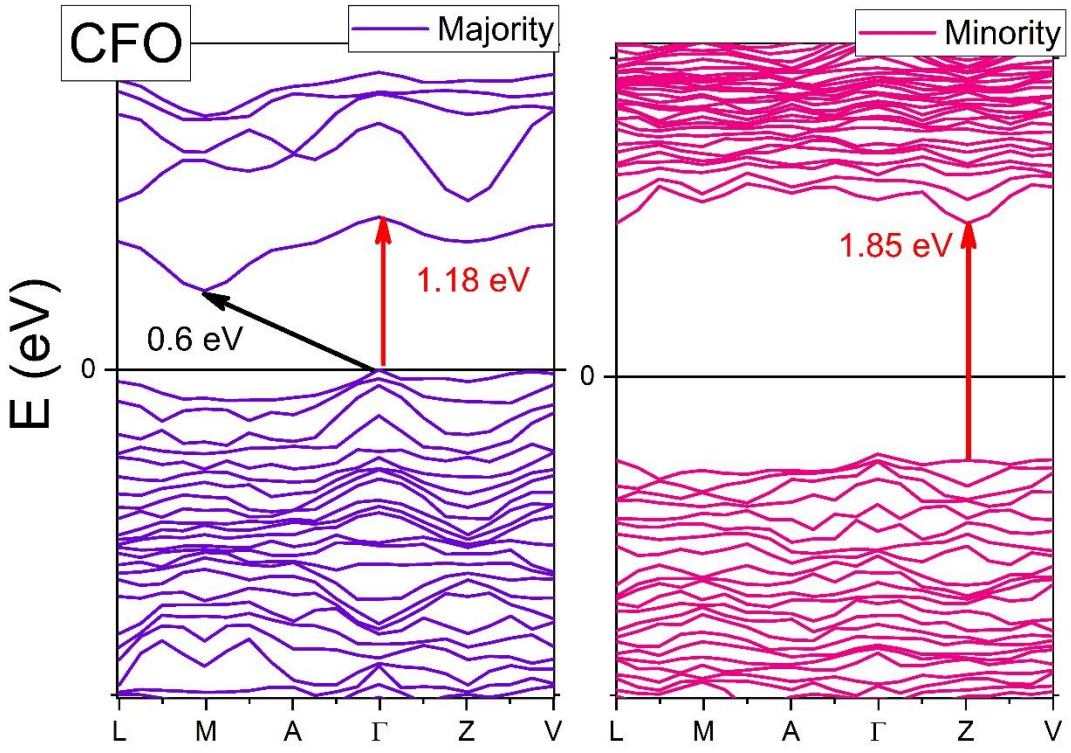

Figure S-I The Zoomed-in image of the bandgap for CFO.

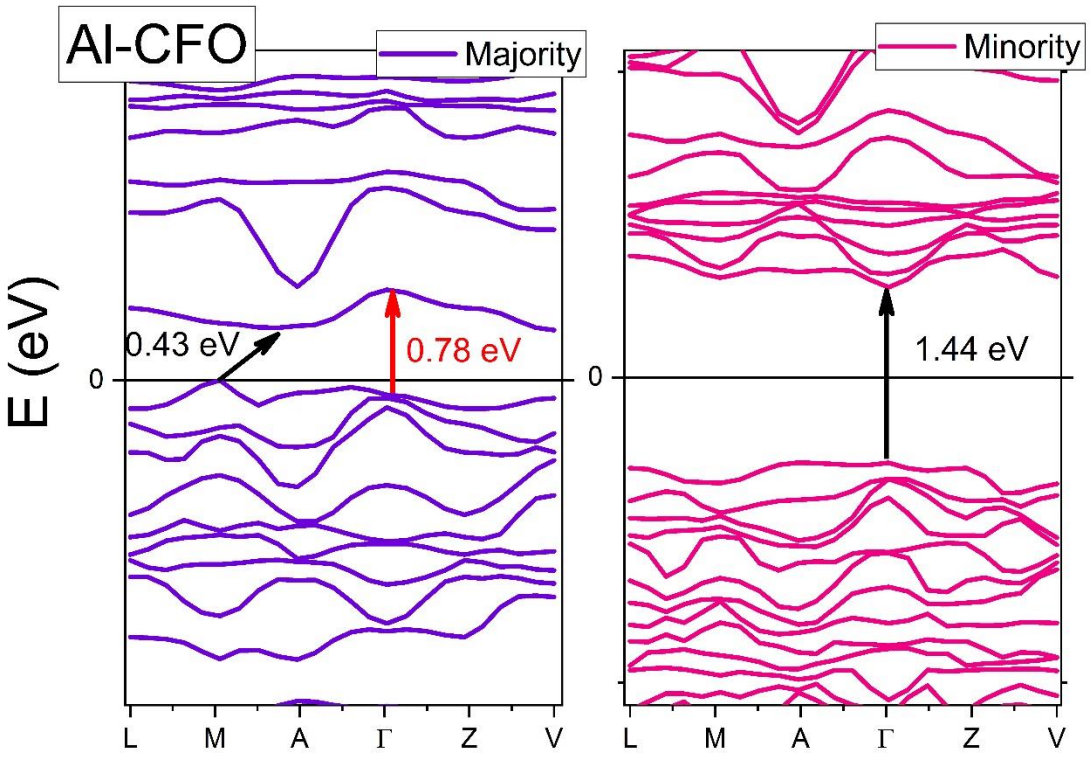

Figure S-II The Zoomed-in image of the bandgap for Al-CFO.

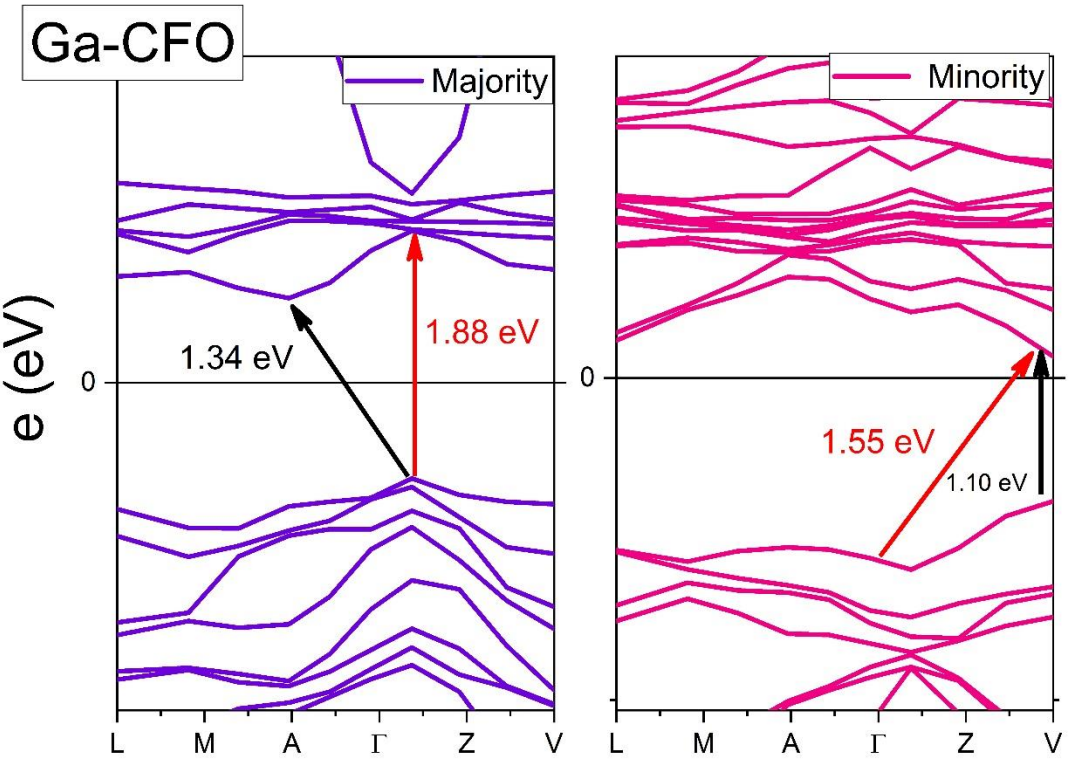

Figure S-III The Zoomed-in image of the bandgap for Ga-CFO.

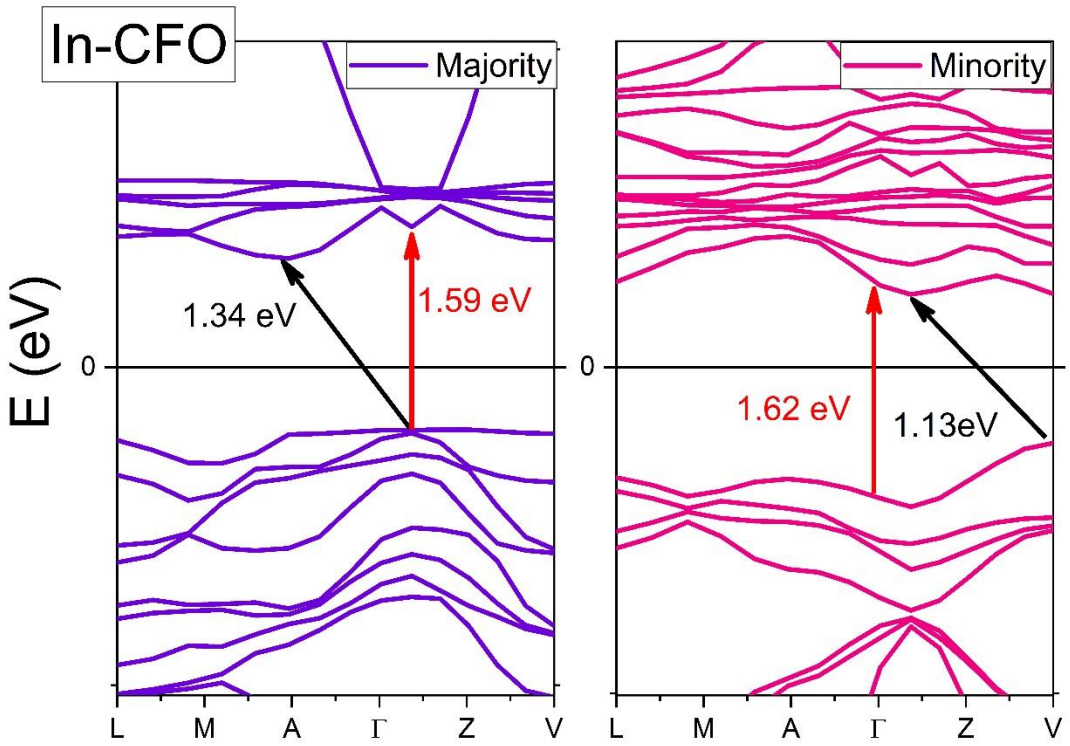

Figure S-IV The Zoomed-in image of the bandgap for In-CFO.

Table S1: Hirschfeld spin moments of individual ions for CFO.

Ion	**Spin Moment (μ_B)**
O1	0.18
O2	0.23
O3	0.23
O4	0.18
O5	0.18
O6	0.23
O7	0.23
O8	0.18
O9	0.13
O10	0.14
O11	0.33
O12	0.11
O13	0.13
O14	0.3
O15	0.15
O16	0.13
Fe1	4.09
Fe2	4.09
Fe3	4.09
Fe4	4.09
Fe5	-3.64
Fe6	-3.61
Fe7	4.1
Fe8	-3.65
Co1	1.97
Co2	1.99
Co3	-2.55
Co4	1.99

Table S2: Hirschfeld spin moments of individual ions for Al-CFO.

Ion	**Spin Moment (μ_B)**
O1	0.14
O2	0.12
O3	0.11
O4	0.11
O5	0.14
O6	0.21
O7	0.17
O8	0.15
Al1	0.04
Fe1	4.07
Fe2	4.07
Fe3	-3.62
Co1	-2.58
Co2	1.89

Table S3: Hirschfeld spin moments of individual ions for Ga-CFO.

Ion	**Spin Moment (μ_B)**
O1	0.24
O2	0.05
O3	0.24
O4	0.05
O5	0.27
O6	0.27
O7	0.14
O8	0.14
Fe1	-3.84
Fe2	4.06
Fe3	4.06
Co1	2.61
Co2	2.61
Ga1	0.1

Table S4: Hirschfeld spin moments of individual ions for In-CFO.

Ion	Spin Moment (μ_B)
O1	0.26
O2	0.05
O3	0.26
O4	0.05
O5	0.3
O6	0.3
O7	0.11
O8	0.11
Fe1	-3.81
Fe2	4.05
Fe3	4.05
Co1	2.58
Co2	2.58
In1	0.11

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