Electronic Supplementary Information – First-principles study on structural, electronic, magnetic and optical properties of lithium zinc ferrite $Li_{1-x}Zn_{2x}Fe_{5-x}O_8$

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Table S1. Lattice constants (a) and total magnetization (M_{tot}) per formula unit (fu) in $Li_{1-x}Zn_{2x}Fe_{5-x}O_8$ (x = 0, 0.25, 0.5, 0.75, 1) with ferrimagnetic (FIM) or antiferromagnetic (AFM) order.

Compound	x	Magnetic order	a (Å)	M_{tot} (μ_B/fu)
LFO	0	FIM	8.302	2.48
LZFO-1	0.25	FIM	8.333	3.82
LZFO-2	0.5	FIM	8.362	4.16
LZFO-3	0.75	FIM	8.386	0.59
ZFO	1.0	AFM	8.417	0.00

Table S2. Number of metal cations at A and B sites in the unit cell for Li-Zn ferrites $(Zn_xFe_{1-x})^A(Li_{(1-x)/2}Fe_{(3+x)/2})^BO_4$ (x = 0, 0.25, 0.5, 0.75, 1).

	x	Zn_A	Fe_A	Fe_B	Li_B
LFO	0	0	8	12	4
LZFO-1	0.25	2	6	13	3
LZFO-2	0.5	4	4	14	2
LZFO-3	0.75	6	2	15	1
ZFO	1	8	0	16	0

Table S3. DFT total energies (E_{tot}) of non-magnetic (NM), ferromagnetic (FM) and antiferromagnetic (AFM) phases, the nearest neighbours (nn) for AB′ ($n_{AB'}$), B′A ($n_{B'A}$) and B′B″ ($n_{B'B''}$) pairs, and Fe ion numbers in A (L_A), B′ ($L_{B'}$) and B″ ($L_{B''}$) sublattices for $Li_{1-x}Zn_{2x}Fe_{5-x}O_8$ (x = 0, 0.25, 0.5 0.75, 1.0).

		E_{tot} (Ry)			nn numbers			Fe numbers		
	x	NM	FM	AFM	$n_{AB'}$	$n_{B'A}$	$n_{B'B''}$	L_A	$L_{B'}$	$L_{B''}$
LFO	0	-6097.811503	-6100.605220	-6101.056630	4.500	6.000	2.2500	8	12	0
LZFO-1	0.25	-6756.454446	-6759.106832	-6759.448410	4.875	4.500	2.4375	6	7	6
LZFO-2	0.5	-7415.174267	-7417.658921	-7417.886246	5.250	3.000	2.6250	4	7	7
LZFO-3	0.75	-8073.901999	-8076.194359	-8076.288529	5.625	1.500	2.8125	2	8	7
ZFO	1	-8732.645535	-8734.791745	-8734.823662	6.000	0.000	3.0000	0	0	16

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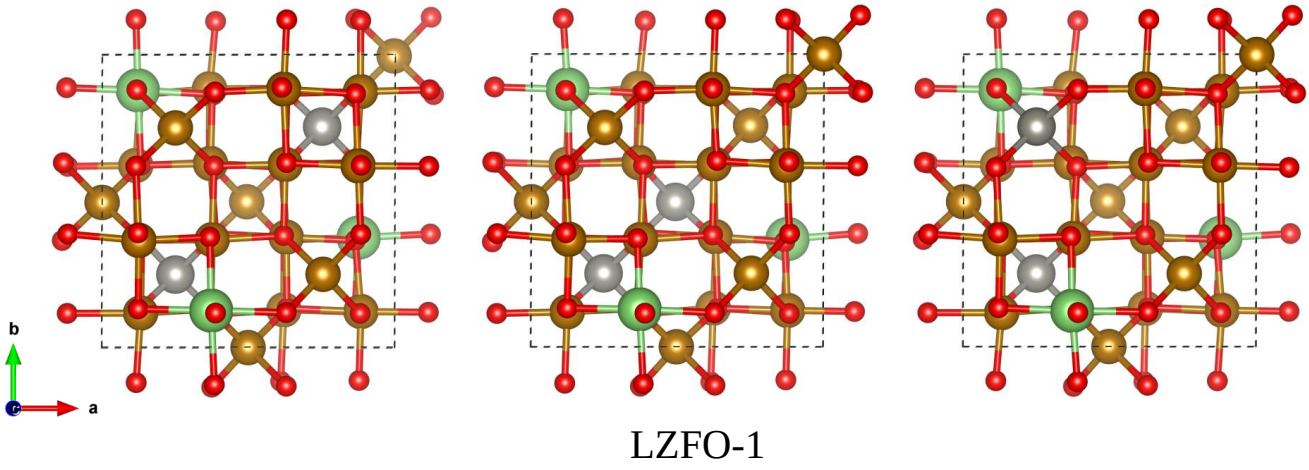

Fig. S1 Ball-and-stick views for possible crystalline structures of LZFO-1 ($Li_{0.75/2}Zn_{0.25}Fe_{4.75/2}O_4$). The green, brown and red balls stand for Li, Fe and O atoms, respectively.

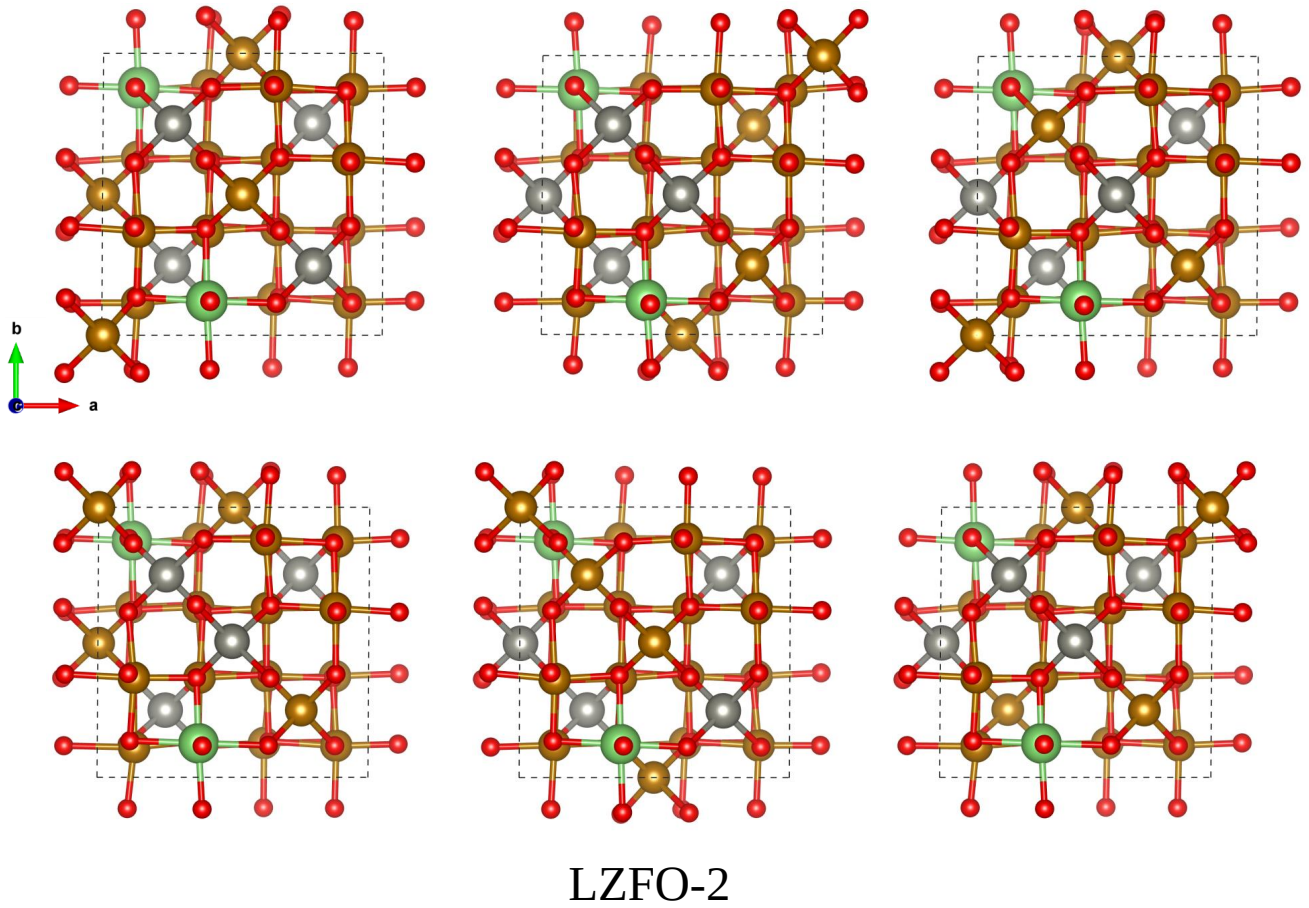

Fig. S2 Ball-and-stick views for possible crystalline structures of LZFO-2 ($Li_{0.5/2}Zn_{0.5}Fe_{4.5/2}O_4$). The green, brown and red balls stand for Li, Fe and O atoms, respectively.

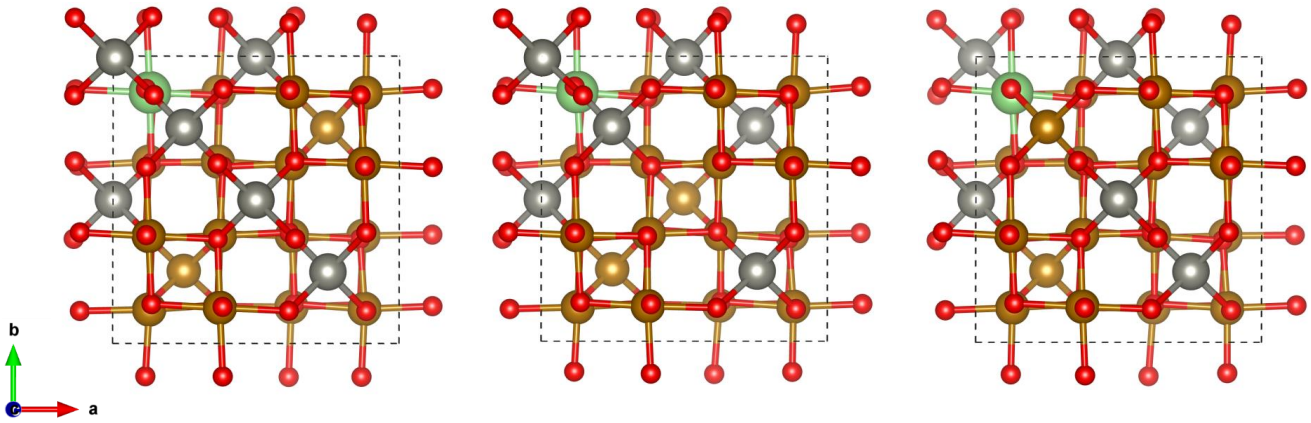

Fig. S3 Ball-and-stick views for possible crystalline structures of LZFO-3 ($Li_{0.25/2}Zn_{0.75}Fe_{4.25/2}O_4$). The green, brown and red balls stand for Li, Fe and O atoms, respectively.

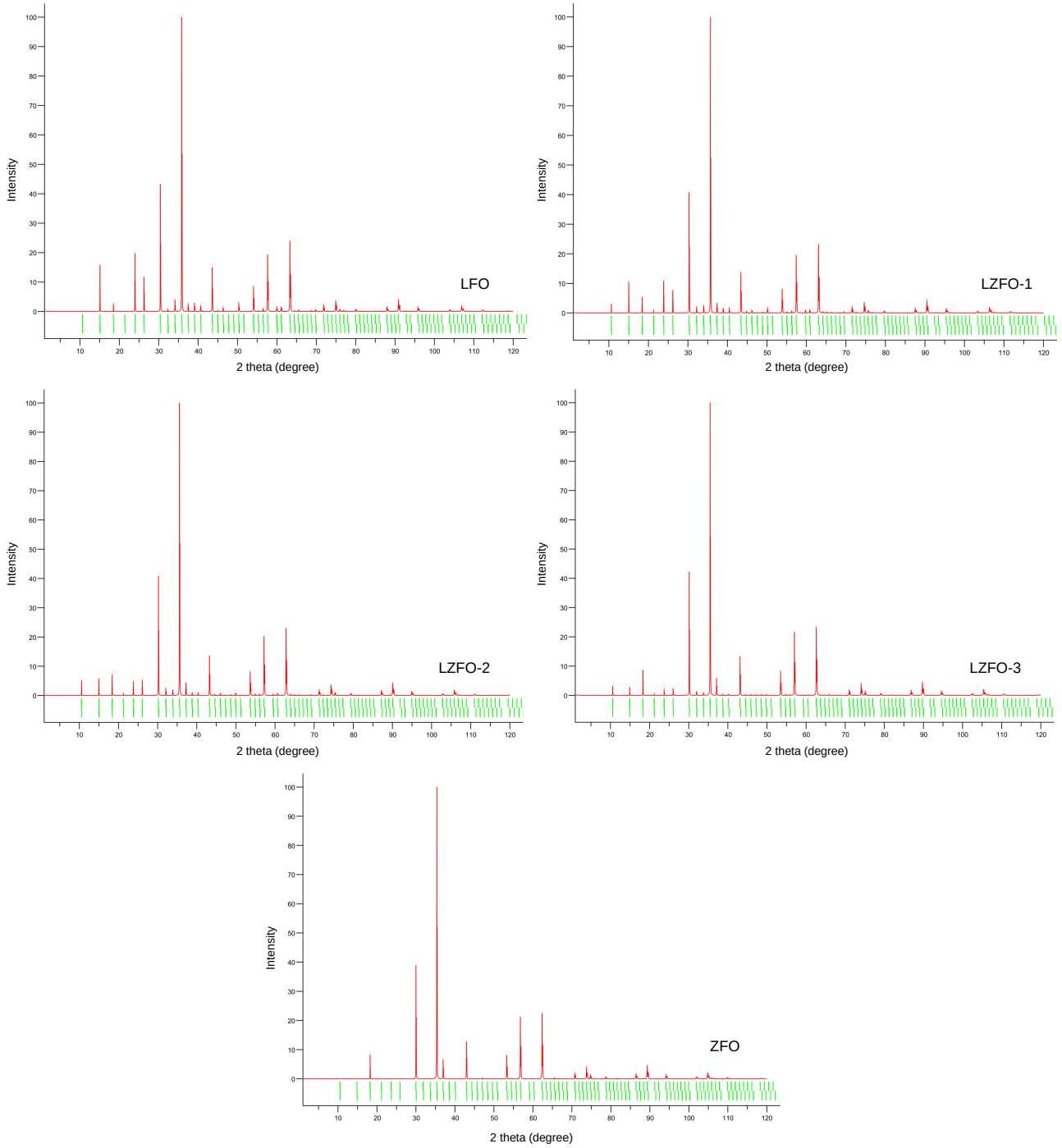

Fig. S4 X-ray diffraction patterns of optimized unit cells for Li–Zn ferrites $Li_{1-x}Zn_{2x}Fe_{5-x}O_8$ (x = 0, 0.25, 0.5, 0.75, 1) simulated by using the VESTA code.

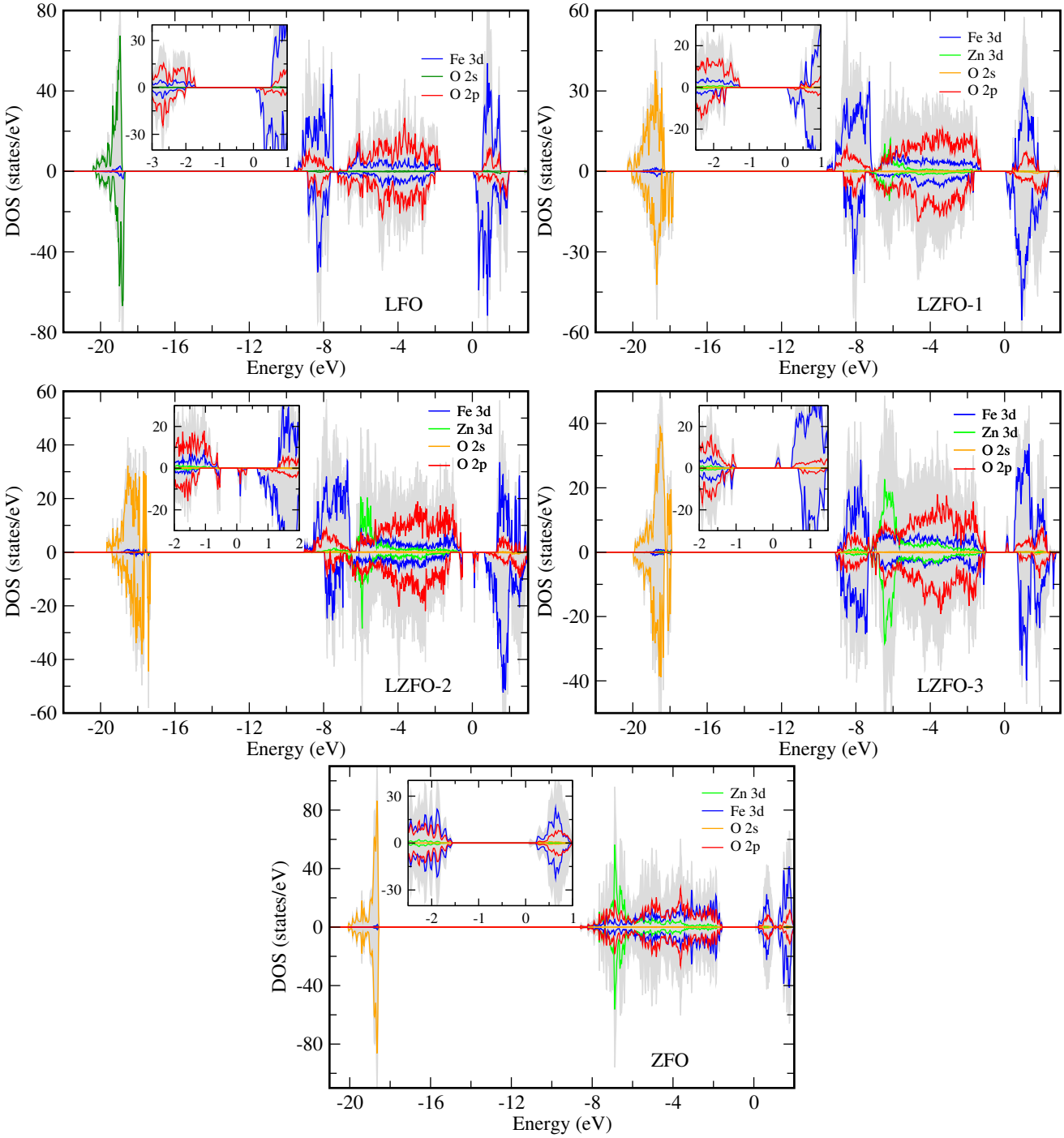

Fig. S5 Atom-projected density of states for $Li_{1-x}Zn_{2x}Fe_{5-x}O_8$ (x = 0, 0.25, 0.5 0.75, 1), where positive values indicate spin up states and negative ones represent spin down states.

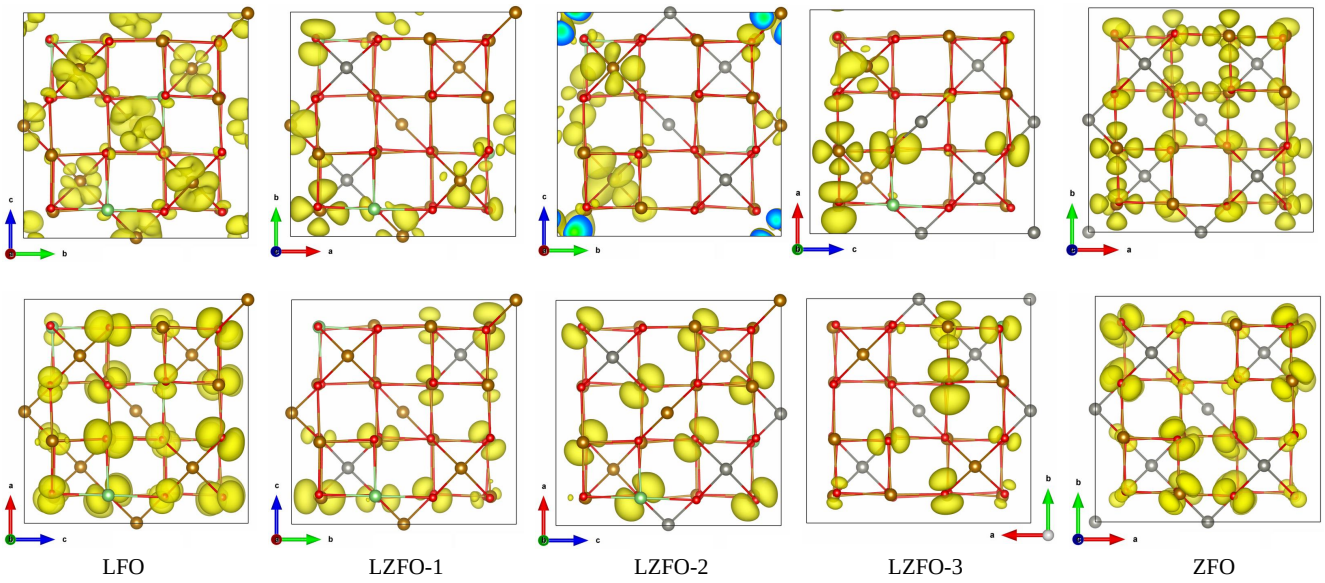

Fig. S6 Squared wave functions corresponding conduction band minimum (top) and valence band maximum (bottom) for spin up configuration in $Li_{1-x}Zn_{2x}Fe_{5-x}O_8$ (x = 0, 0.25, 0.5 0.75, 1).

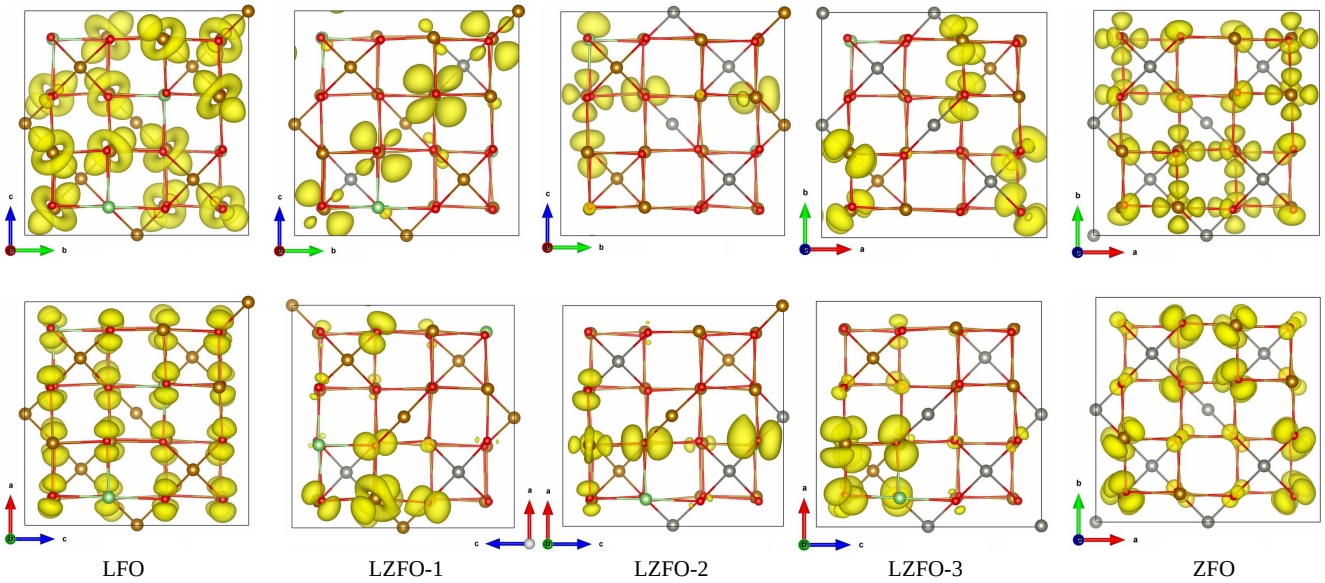

Fig. S7 Squared wave functions corresponding conduction band minimum (top) and valence band maximum (bottom) for spin down configuration in $Li_{1-x}Zn_{2x}Fe_{5-x}O_8$ (x = 0, 0.25, 0.5 0.75, 1).

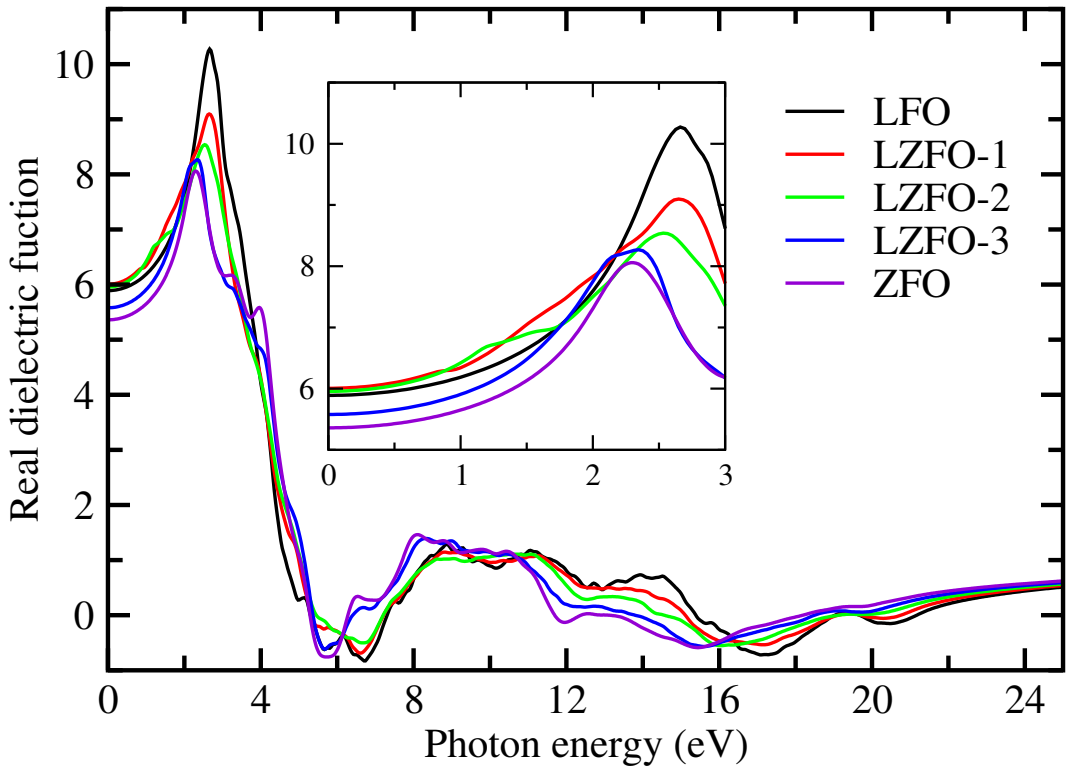

Fig. S8 Real part of frequency-dependent dielectric function $\varepsilon(\omega)$ in $Li_{1-x}Zn_{2x}Fe_{5-x}O_8$ (x = 0, 0.25, 0.5 0.75, 1).

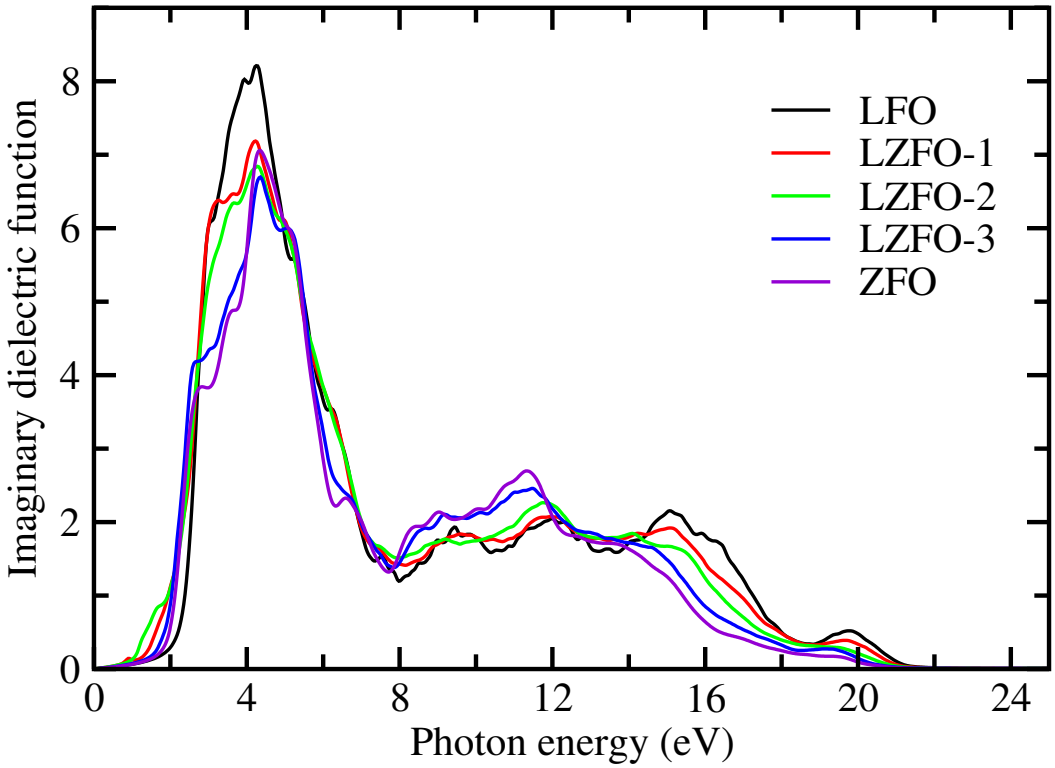

Fig. S9 Imaginary part of frequency-dependent dielectric function $\varepsilon(\omega)$ in $Li_{1-x}Zn_{2x}Fe_{5-x}O_8$ (x = 0, 0.25, 0.5 0.75, 1).

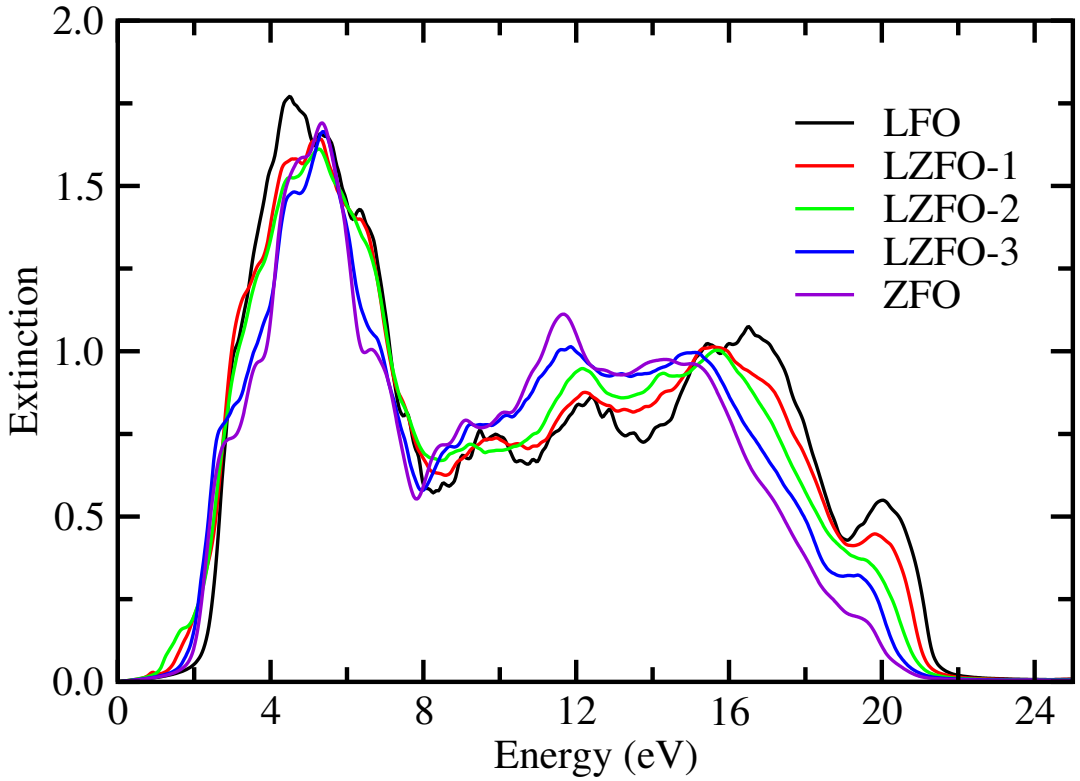

Fig. S10 Extinction coefficient in $Li_{1-x}Zn_{2x}Fe_{5-x}O_8$ (x = 0, 0.25, 0.5 0.75, 1).