Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information

Strongly-bound Wannier-Mott Exciton in Pristine (LaO)MnAs and Origin of Ferrimagnetism in F-doped (LaO)MnAs

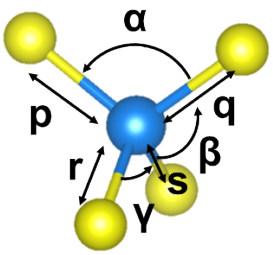
Jessie Manopo[a, b], Tio Prince Lubis[a, b], Muhammad Arief Mustajab Enha Maryono[b], Pepen Arifin[b], Toto Winata[b], Rena Widita[c], and Yudi Darma[a, b]†

[a]Quantum Semiconductor and Devices Lab., Department of Physics, Faculty of Mathematics and Natural Sciences, Bandung Institute of Technology, Jalan Ganesha 10 Bandung, 40132, Indonesia.

[b]Physics of Electronic Materials Research Division, Department of Physics, Faculty of Mathematics and Natural Sciences, Bandung Institute of Technology, Jalan Ganesha 10 Bandung, 40132, Indonesia.

[c] Nuclear Physics and Biophysics Research Division, Department of Physics, Faculty of Mathematics and Natural Sciences, Bandung Institute of Technology, Jalan Ganesha 10 Bandung, 40132, Indonesia

Table S1. Bond lengths and angles of $MnAs_4$ tetrahedra in pristine and doped (LaO)MnAs

	α	β	p (Å)	q (Å)	r (Å)	s (Å)	γ	Illustration
pristine	106.962	110.74	2.5592	2.5592	2.5592	2.5592	106.962	
6.25%	106.54	110.815	2.5612	2.5612	2.5696	2.5696	107.088	
	106.957	110.702	2.5559	2.5586	2.5641	2.5652	106.514	
12.50%	106.53	111.124	2.5618	2.5627	2.5627	2.5618	106.53	
	105.787	111.344	2.5594	2.5594	2.5594	2.5594	105.787	
25%	106.935	111.362	2.5445	2.5445	2.5850	2.5850	104.544 (Mn2)	
	106.444	111.369	2.5526	2.5526	2.5767	2.5767	105.024 (Mn1)	

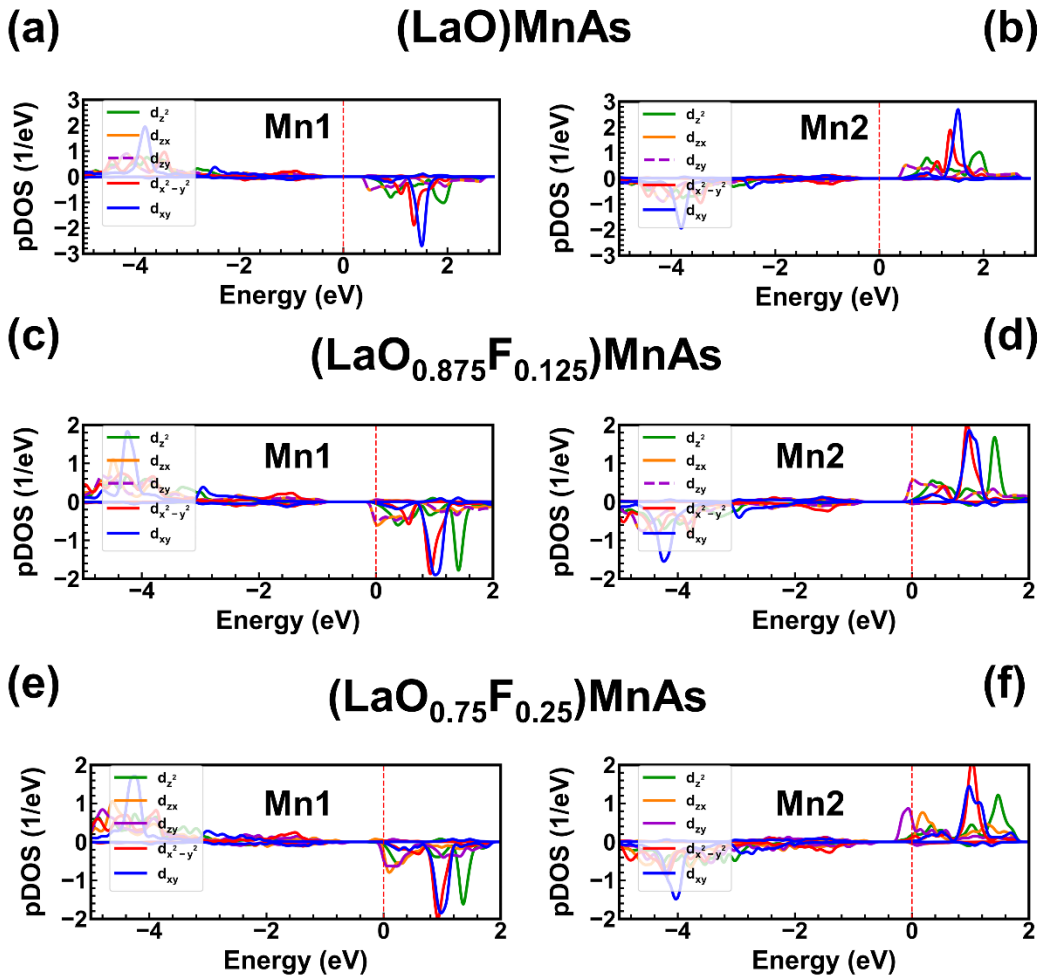


Figure S1. Calculated projected density of states for (a) Mn1 and (b) Mn2 d orbital of pristine (LaO)MnAs, (c) Mn1 and (d) Mn2 d orbital of ($LaO_{0.875}F_{0.125}$), (e) Mn1 and (f) Mn2 d orbital of ($LaO_{0.75}F_{0.25}$)MnAs.

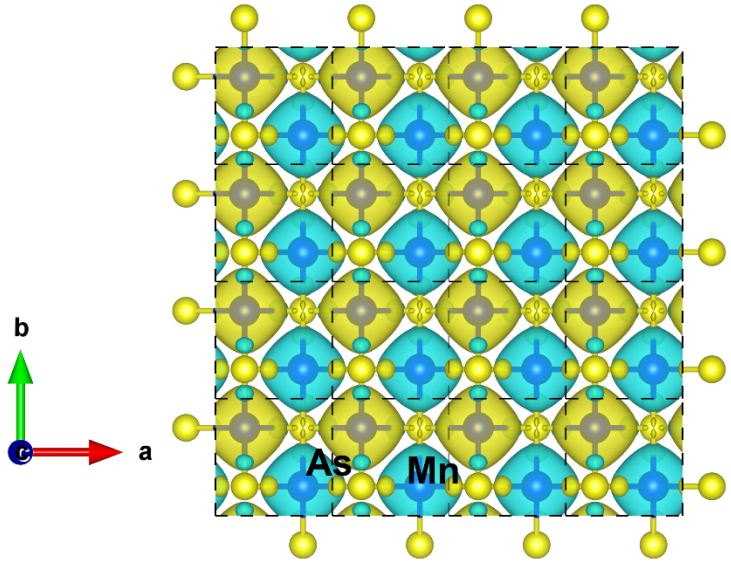


Figure S2. Calculated spin charge density of (MnAs) layer of ($LaO_{0.75}F_{0.25}$)MnAs with isosurface level of 0.003 eV/Å, where yellow and blue isosurfaces denote spin up and down respectively.

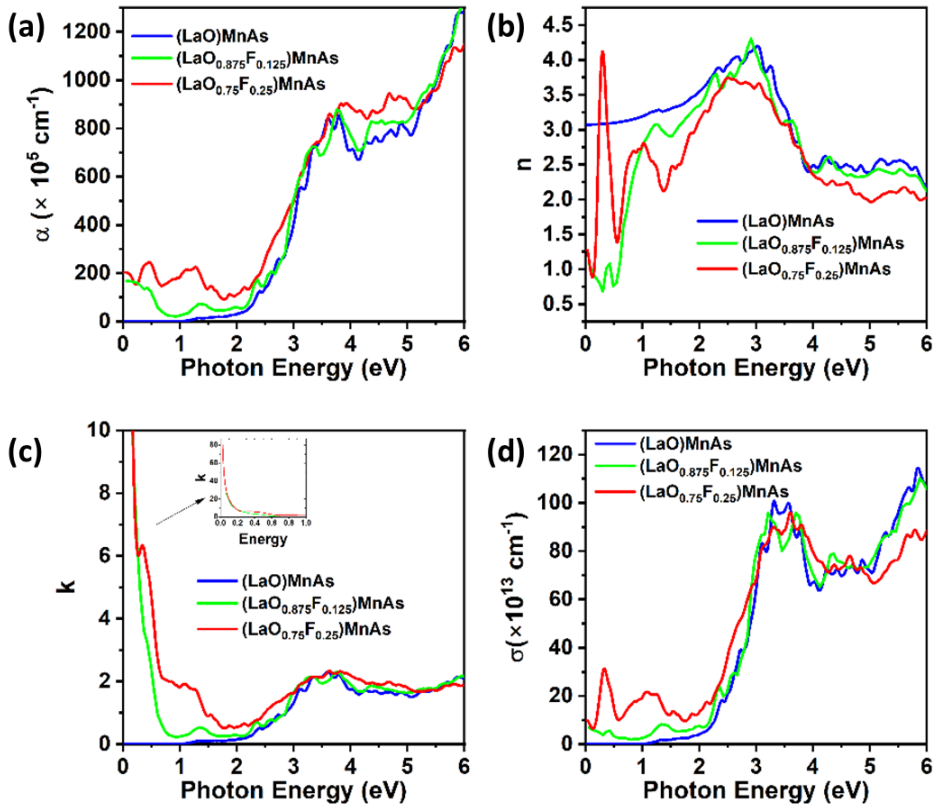


Figure S3. Calculated (a) absorption coefficient, (b) refractive index, (c) extinction coefficient, and (d) optical conductivity of pristine (LaO)MnAs, $(LaO_{0.875}F_{0.125})$MnAs, and $(LaO_{0.75}F_{0.25})$MnAs.

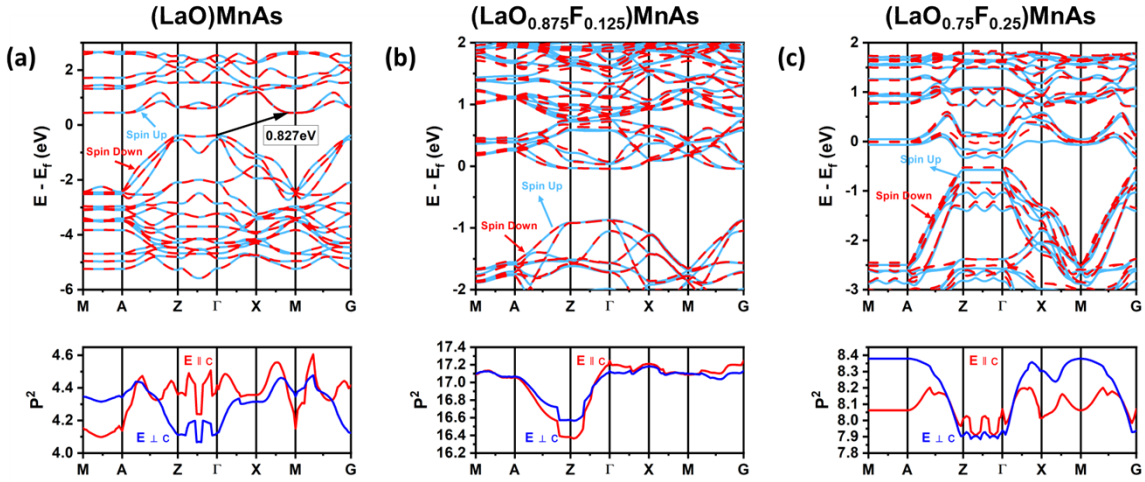


Figure S4. Momentum matrix elements of (a) pristine (LaO)MnAs, (b) $(LaO_{0.875}F_{0.125})$MnAs, (c) and $(LaO_{0.75}F_{0.25})$MnAs.