

# Supplementary material for “Magnetic charge and the magnetoelectricity in hexagonal manganites $RMnO_3$ and ferrites $RFeO_3$ ”

Meng Ye and David Vanderbilt

*Department of Physics & Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*

In Tables II-III of the main text, we provided detailed information on the Born charge tensors and force constant eigenvalues only for the two representative materials  $LuMnO_3$  and  $LuFeO_3$ . Here, we provide the same information for the other materials covered by this study. Note that the values given in the last two columns of each table are redundant with those given in Tables II-III of the main text.

TABLE I: Atomic Born charge tensors  $Z^e$  (in units of  $|e|$ ) for  $RMnO_3$  and  $LuFeO_3$  in the  $A_2$  phase. TM = Mn, Fe.

	HoMnO <sub>3</sub>	ErMnO <sub>3</sub>	YbMnO <sub>3</sub>	LuMnO <sub>3</sub>	LuFeO <sub>3</sub>
$Z_{xx}^e(R_1)$	3.69	3.67	3.62	3.61	3.79
$Z_{zz}^e(R_1)$	4.16	4.15	4.11	4.12	3.94
$Z_{xx}^e(R_2)$	3.76	3.73	3.67	3.66	3.84
$Z_{yx}^e(R_2)$	0.13	0.13	0.13	0.13	0.15
$Z_{zz}^e(R_2)$	4.07	4.05	4.00	3.96	3.88
$Z_{xx}^e(TM)$	3.16	3.17	3.17	3.17	2.96
$Z_{zz}^e(TM)$	0.41	0.42	0.43	0.44	0.21
$Z_{yy}^e(TM)$	3.25	3.25	3.26	3.26	3.01
$Z_{xz}^e(TM)$	0.07	0.07	0.07	0.07	-0.02
$Z_{zz}^e(TM)$	4.02	4.01	3.97	3.95	4.16
$Z_{xx}^e(O_{T1})$	-1.95	-1.94	-1.92	-1.92	-2.19
$Z_{xx}^e(O_{T1})$	0.24	0.24	0.24	0.25	0.25
$Z_{yy}^e(O_{T1})$	-2.05	-2.03	-2.00	-2.00	-2.28
$Z_{xz}^e(O_{T1})$	0.19	0.19	0.19	0.19	0.11
$Z_{zz}^e(O_{T1})$	-3.24	-3.24	-3.20	-3.19	-3.21
$Z_{xx}^e(O_{T2})$	-1.95	-1.93	-1.91	-1.90	-2.15
$Z_{zx}^e(O_{T2})$	-0.20	-0.20	-0.20	-0.20	-0.19
$Z_{yy}^e(O_{T2})$	-1.88	-1.87	-1.85	-1.85	-2.13
$Z_{xz}^e(O_{T2})$	-0.18	-0.18	-0.18	-0.18	-0.11
$Z_{zz}^e(O_{T2})$	-3.38	-3.38	-3.34	-3.33	-3.30
$Z_{xx}^e(O_{P1})$	-3.01	-3.01	-3.01	-3.00	-2.40
$Z_{zz}^e(O_{P1})$	-1.58	-1.57	-1.54	-1.54	-1.61
$Z_{xx}^e(O_{P2})$	-3.05	-3.05	-3.06	-3.05	-2.45
$Z_{yx}^e(O_{P2})$	-0.03	-0.03	-0.03	-0.03	-0.02
$Z_{zz}^e(O_{P2})$	-1.47	-1.46	-1.43	-1.43	-1.52

TABLE II: Eigenvalues of the force-constants matrix ( $eV/\text{\AA}^2$ ) for IR-active modes in  $RMnO_3$  and  $LuFeO_3$  in the  $A_2$  phase, and for  $HoMnO_3$  in the  $A_1$  phase

	HoMnO <sub>3</sub>	ErMnO <sub>3</sub>	YbMnO <sub>3</sub>	LuMnO <sub>3</sub>	LuFeO <sub>3</sub>
Longitudinal $A_1$ modes					
	4.23	4.23	4.25	4.24	3.48
	7.11	7.18	7.35	7.44	6.70
	8.14	8.27	8.60	8.74	8.41
	10.77	10.90	11.34	11.51	11.47
	13.69	13.82	13.98	14.01	12.03
	14.85	15.03	15.42	15.60	15.59
	21.32	21.60	22.36	22.66	20.53
	25.44	25.57	25.67	25.87	22.83
	35.99	35.68	35.54	35.82	28.46
Transverse $E_1$ modes					
	3.23	3.37	3.27	3.32	3.56
	4.22	4.25	4.49	4.68	4.62
	5.96	6.28	6.63	6.73	6.97
	7.59	6.93	7.01	7.35	8.09
	8.41	8.56	8.57	8.63	8.83
	9.29	8.99	9.31	9.56	9.24
	9.65	10.12	10.95	11.36	11.37
	11.23	11.25	12.02	12.46	12.46
	12.57	12.85	12.95	13.02	13.85
	13.29	13.54	13.77	14.09	14.92
	16.41	16.76	16.57	16.49	16.87
	17.49	17.52	17.38	17.37	17.35
	22.79	23.02	23.16	23.36	21.19
	36.18	37.99	37.54	37.75	28.75