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Spontaneous electric polarization and electric field gradient in hybrid improper ferroelectrics: insights and correlations

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Supplementary information

Figure S1 shows the asymmetry parameter (η) as a function of the spontaneous electric polarization squared (P^2) for the $Ca_3Mn_2O_7$ system. At $P = 0$ the data correspond to the paraelectric *Cmcm* and *Cmce* phases and at $P^2 = 26.94$ $(\mu C/cm^2)^2$ to the ferroelectric $A2_1am$ phase.

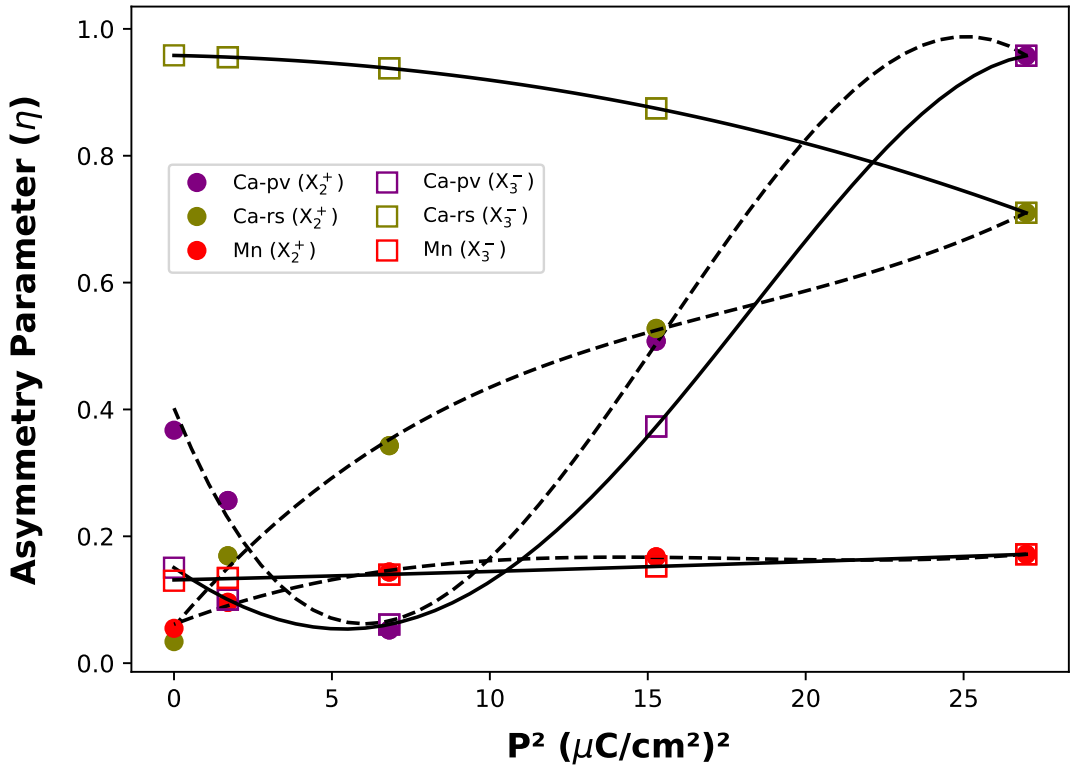

Figure S1: Asymmetry parameter (η) for the $Ca_3Mn_2O_7$ system at sites A (Ca-pv), A′ (Ca-rs), and B (Mn atom).

Figures S2, S3, and S4 show, respectively, the $g(\theta,\phi)$ surface plot of the $Ca_3Ti_2O_7$, $Cd_3Mn_2O_7$, and $Cd_3Ti_2O_7$ systems.

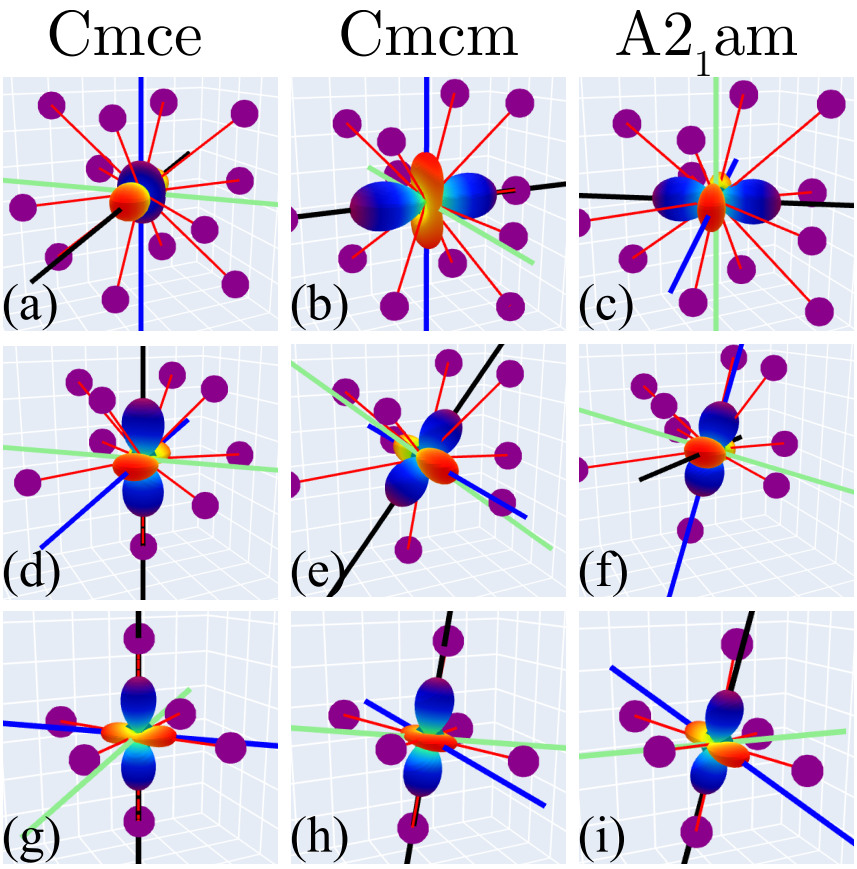

Figure S2: $g(\theta,\phi)$ surface plot of the $Ca_3Ti_2O_7$ compound for the polar $A2_1am$, and the centrosymmetric *Cmcm* and *Cmce* space groups along the X_2^+ and X_3^- paths, respectively. (a-c) at Ca rs-site (A′-site), (d-f) at Ca pv-site (A-site), and (g-i) at Ti-site (B-site). The green, blue, and black axes represent the directions of the V_{xx}, V_{yy}, and V_{zz} EFG components, respectively. Blue color regions depict where the polar function is negative and red color regions where it is positive.

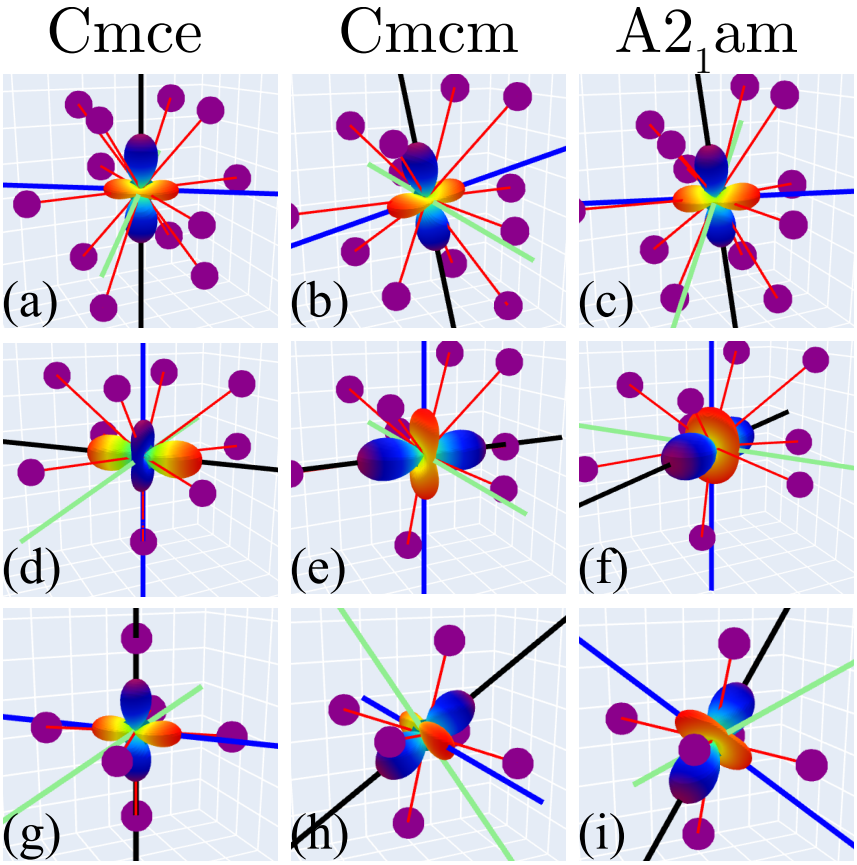

Figure S3: $g(\theta,\phi)$ surface plot of the $Cd_3Mn_2O_7$ compound for the polar $A2_1am$, and the centrosymmetric *Cmcm* and *Cmce* space groups along the X_2^+ and X_3^- paths, respectively. (a-c) at Cd rs-site (A′-site), (d-f) at Cd pv-site (A-site), and (g-i) at Mn-site (B-site). The green, blue, and black axes represent the directions of the V_{xx}, V_{yy}, and V_{zz} EFG components, respectively. Blue color regions depict where the polar function is negative and red color regions where it is positive.

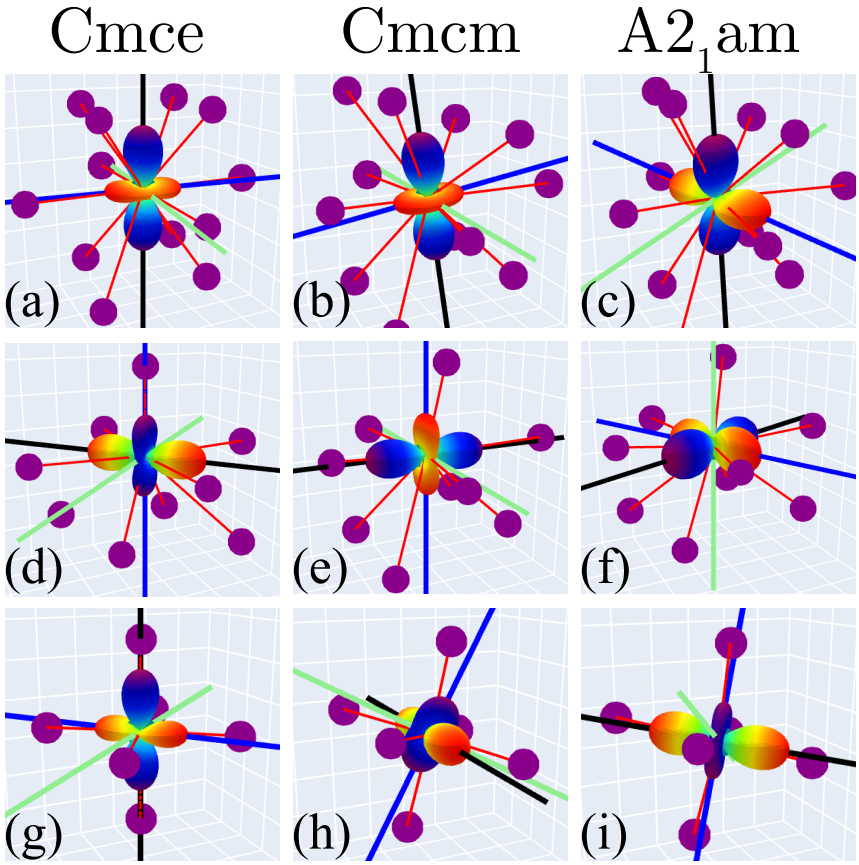

Figure S4: $g(\theta,\phi)$ surface plot of the $Cd_3Ti_2O_7$ compound for the polar $A2_1am$, and the centrosymmetric *Cmcm* and *Cmce* space groups along the X_2^+ and X_3^- paths, respectively. (a-c) at Cd rs-site (A′-site), (d-f) at Cd pv-site (A-site), and (g-i) at Ti-site (B-site). The green, blue, and black axes represent the directions of the V_{xx}, V_{yy}, and V_{zz} EFG components, respectively. Blue color regions depict where the polar function is negative and red color regions where it is positive.