Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Cadmium-based ferroelectrics with the Ruddlesden-Popper and double perovskite structures: a theoretical study

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Supplementary Information

Here we show the effect of spin-orbit coupling in the electronic and ferroelectric properties of Cd-based structures. Figure S1 compares the bandstructures of $CaCd_2Mn_2O_7$ and $CaCd_2Ti_2O_7$ with and without SOC. Most of the effects of SOC are concentrated on the conduction band. Ferroelectricity is caused by a displacement of the center of Wannier functions with respect to the positive charges. Because only occupied orbitals are important for the polarization, changes in the conduction band would cause only minor effects, as shown in Table S1, which compares the electric polarization with and without SOC.

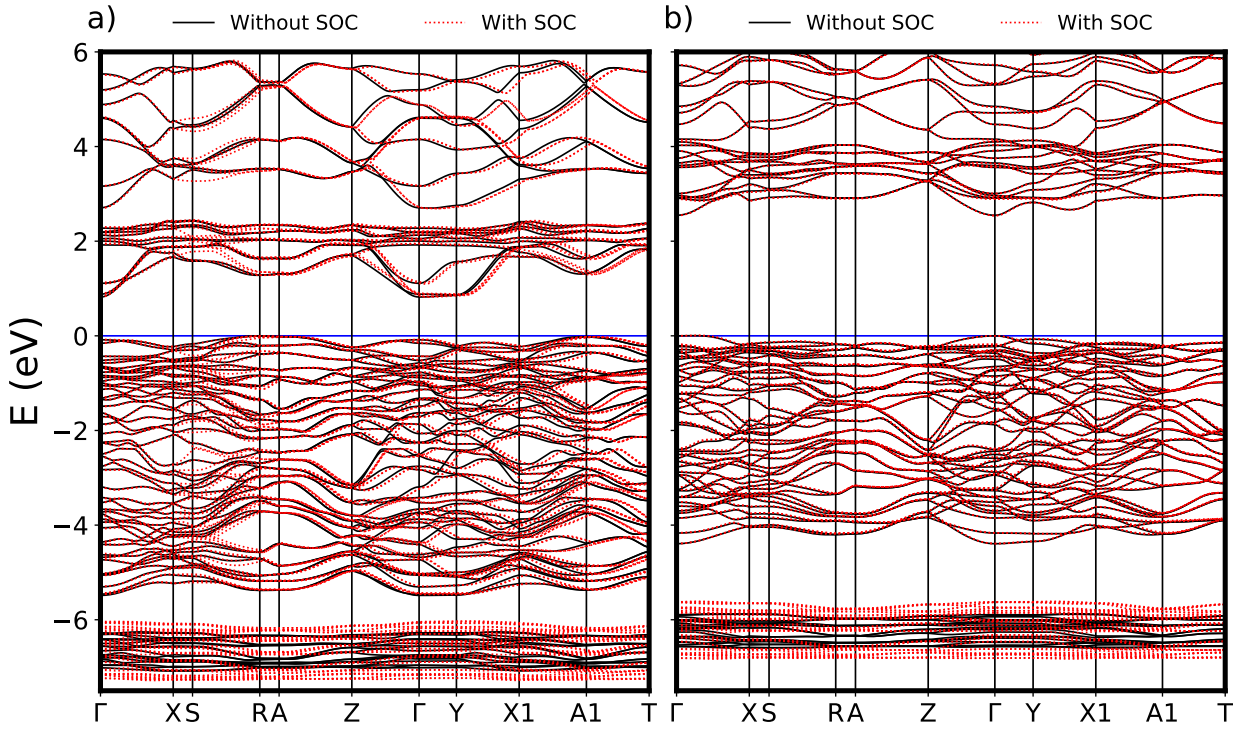

Figure S1 - Band structures of $CaCd_2Mn_2O_7$ (a) and $CaCd_2Ti_2O_7$ (b) with and without spin-orbit coupling (SOC)

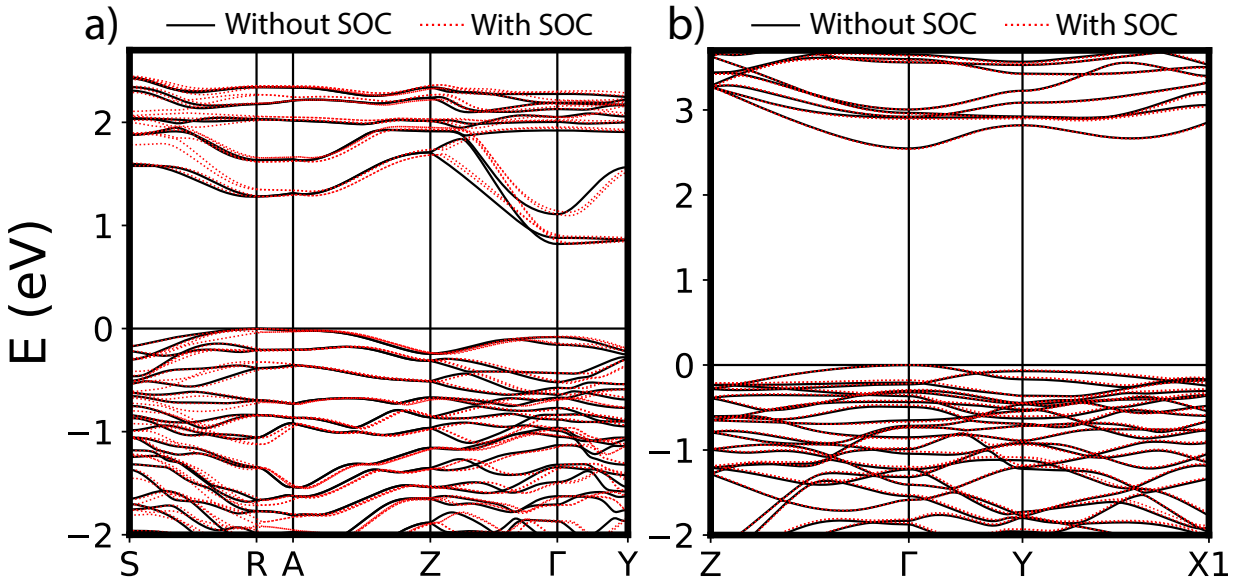

Figure S2 - Details around the Fermi energy of the bandstructures of $CaCd_2Mn_2O_7$ (a) and $CaCd_2Ti_2O_7$ (b). For Mn systems, most changes due to spin-orbit coupling are in the conduction band. SOC does not affect the bandstructure of the Ti compound.

Table S1 - Comparison between the electric polarization computed with and without spin-orbit coupling (SOC). The values are slightly different from those of Table 5 of the article because here we used norm conserving pseudopotentials.

Polarization ($\mu C/cm^2$)		
Crystal	**Without SOC**	**SOC**
$Cd_3Ti_2O_7$	44.73	44.72
$Cd_3Mn_2O_7$	9.61	9.60
$CaCd_2Mn_2O_7$	6.14	6.15
$CaCdMn_2O_6$	4.09	4.08
$Ca_3Mn_2O_7$	5.00	5.00
$Ca_3Ti_2O_7$	26.86	26.86
$CaCd_2Ti_2O_7$	19.34	19.34