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Density functional study of the spin exchange interactions, magnetic structures and ferroelectric polarizations of multiferroics driven by magnetic order

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The electronic structures of magnetic insulators LiCuVO_4 , LiCu_2O_2 , TbMnO_3 , $\text{Ca}_3\text{CoMnO}_6$, MnWO_4 , CuFeO_2 , $\text{Ba}_2\text{CoGe}_2\text{O}_7$ and CuBr were examined on the basis of first principles DFT+U+SOC calculations to evaluate their spin exchange parameters and account for their ordered magnetic structures. We then explored how the electric polarizations of these compounds are related to the magnetic ordering and spin-orbit coupling. In this talk results of our studies will be presented.