

Abstract Submitted
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Magnetoelectric response of LiNiPO_4 from first-principles ERIC BOUSQUET, UCSB, NICOLA SPALDIN, PHILIPPE GHOSEZ, MATERIALS DEPARTMENT UCSB TEAM, LIEGE UNIVERSITY TEAM — The lithium orthophosphates LiMPO_4 ($M = \text{Mn, Fe, Co, Ni}$) have attracted large interest because of their potential use in cathode electrode for Li-ion batteries as well as their large magnetoelectric response and more recently because of the presence of ferrotoroidic domains in LiCoPO_4 . Here we will discuss the response to a static magnetic field of LiNiPO_4 by means of first-principles calculations. This will allow us to extract the magnetic susceptibility as well as the magnetoelectric coefficients and to analyze their microscopic origin by decomposing the electronic and the ionic contributions. This last decomposition highlight the importance of the electronic contribution to the magnetoelectric response.

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