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Large dynamical magnetic charges driven by exchange striction
MENG YE, DAVID VANDERBILT, Rutgers University - New Brunswick — Magnetoelectric (ME) materials are of fundamental interest and are investigated for their broad potential applications. First-principles methods have only recently been developed to calculate the full ME response tensor α including both electronic and ionic contributions.[1] In several materials, the dominant contribution to the ME response has been shown to be the ionic term $\alpha_{\rm ion}$, which is proportional to both the Born charge $Z^{\rm e}$ and its analogue, the dynamical magnetic charge $Z^{\rm m}$.[2] Here we present a theoretical study of mechanisms that could enhance the magnetic charge $Z^{\rm m}$. The KITPite structure is reported with large ME response arising from exchange striction and spin frustration.[3] Using first-principles density-functional methods, we calculate the atomic $Z^{\rm m}$ tensors in KITPite and conclude that even when SOC is completely absent, the exchange striction acting on the non-collinear spin structure induces much larger magnetic charges than in the case when $Z^{\rm m}$ is driven by SOC as in Cr_2O_3.

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[2]J. Íñiguez, Phys. Rev. Lett. **101**, 117201 (2008).
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