Large dynamical magnetic charges driven by exchange striction
MENG YE, DAVID VANDERBILT, Rutgers University - New Brunswick — Magnetoelastic (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 $\alpha$ 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 $\alpha_{\text{ion}}$, which is proportional to both the Born charge $Z^e$ and its analogue, the dynamical magnetic charge $Z^m$.\(^2\) Here we present a theoretical study of mechanisms that could enhance the magnetic charge $Z^m$. 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 $Z^m$ 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 $Z^m$ is driven by SOC as in $\text{Cr}_2\text{O}_3$.


Meng Ye
Rutgers University - New Brunswick

Date submitted: 14 Nov 2013

Electronic form version 1.4