Magnetic interactions and excitations in high-T_c three-dimensional Slater insulator $NaOsO_3$

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In contrast to Mott insulating phase found in many correlated systems, the Slater insulator in three dimensions is very rare and has been observed in a handful of compounds. One prominent example is $NaOsO_3$ which undergoes an antiferromagnetic transition at 410 K where a small electronic gap $\sim$0.1 eV is induced [1,2]. Interestingly, the continuous metal-insulator transition in $NaOsO_3$ is challenging even for the state-of-the-art theory. In this work, our goal is to study the magnetic interactions in this $5d$ oxide and to analyze the effect of different theory approximations on the predicted magnetic properties. Our calculations are based on density functional theory where electronic correlations are included on the static mean-field level and the relativistic generalization of the magnetic force theorem, both available in the RSPt electronic structure software [3]. The quality of the theoretical description is assessed by comparing the calculated and measured magnon spectra [4]. We have clarified the role of different types of magnetic interactions, i.e. Heisenberg, Dzyaloshinskii-Moriya and symmetric anisotropic exchange as well as the on-site anisotropy, by disentangling their contributions to the magnetic excitation spectra.

References:

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