

Benchmarking computed and experimental neutron form factors for MnO and NiO

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Sources for neutron scattering have become powerful enough to capture information about the equal time spin-spin correlation function, $S(\mathbf{q})$, which at large values of \mathbf{q} gives information about the microscopic details of the spin density. We use density functional theory, and fixed-node diffusion Monte Carlo to benchmark these methods against the intensity and form factor captured by powder neutron diffraction experiments run at the University of Missouri Research Reactor. These comparisons will allow us to discern the extent to which these methods capture the microscopic details of magnetism in MnO and NiO, and what can potentially be done to adjust the spin-spin correlations.