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Constraints on magnetism and correlations in RuO₂ from inelastic neutron/x-ray scattering and Mössbauer spectroscopy

We provide experimental evidence for the absence of a magnetic moment in bulk RuO₂, a candidate altermagnetic material, by using a combination of inelastic neutron and X-ray scattering, Mössbauer spectroscopy, nuclear forward scattering, and density functional theory calculations. The lattice dynamics from our inelastic neutron/x-ray scattering experiments were compared to density functional theory calculated lattice dynamics with various functionals by estimating the dynamic structure factor and the bose-factor corrected dynamic susceptibility. This comparison reveals that the DFT calculated non-magnetic RuO₂ structure provides the best description of our inelastic scattering experiments. Using complementary Mössbauer and nuclear forward scattering we also determine the ⁹⁹Ru magnetic hyperfine splitting to be negligible, which further substantiates the non-magnetic behavior of RuO₂. Our comprehensive analysis indicates that the electronic correlations, rather than magnetic order, are key in describing the lattice dynamics.

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Reference

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