

Abstract Submitted
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Ultrafast switching of the magnetic ground state in d^1 titanates through nonlinear phononic coupling¹ MINGQIANG GU, JAMES M RONDINELLI, Northwestern University — LaTiO₃ and YTiO₃ are isostructure d^1 titanates, which exhibit distinct magnetic and orbital properties: The former is a G-type antiferromagnet with a 150 K Neel temperature whereas the latter is a rare ferromagnetic (FM) insulator with a 30 K Curie temperature. With first-principles density functional theory calculations, we identify the local structural origin of the magnetic order difference in these orthorhombic perovskites. By increasing the tilt and rotation angles in LaTiO₃, respectively, LaTiO₃ is predicted to undergo a magnetic phase transition to an FM state. Similarly, decreasing the tilt and rotation angles in YTiO₃ leads to a FM-to-AFM phase transition. The underlying physics is attributed to the change in the superexchange coupling between Ti-sites. Last, we propose a route to switch the magnetism in the titanates by controlling the octahedral distortions through dynamical nonlinear phononic coupling. The proposed experiment requires the use of static strain to position the crystal structure in proximity to the structural transition combined with readily achievable fluencies in an ultrafast optical pump-probe geometry

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Mingqiang Gu
Northwestern University

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