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A new kind of line defect in NdTiO3 perovskite¹ MEHMET TOP-SAKAL, JONG SEOK JEONG, PENG XU, BHARAT JALAN, RENATA WENTZ-COVITCH, ANDRE MKHOYAN, University of Minnesota — We report an observation of a new line defect in strained NdTiO3 perovskite. Aberration-corrected analytical scanning transmission electron microscopy and first-principles calculations are used to characterize its atomic structure and electronic properties. The defect represents a shift and rotation of the core Ti-O-Nd unit accommodating the deficiency of Ti-O units in neighboring columns and strain. The core of the defect has considerably different electronic properties resulting from Ti being in different oxidation states. This observation closes the dimensionality gap between previously observed point and planar defects in complex oxides needed to accommodate the alterations of stoichiometry and strain. This new line defect should also exist in other multi-valent perovskites, and could open a new avenue for tailoring unexpected and highly-desirable electronic properties.

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