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Prediction of novel perovskite-type oxyhydride $KTi(O_2H)$ with two-dimensional electronic states[1] NOBUYA SATO, SHINJI TSUNEYUKI, Dept. of Phys., The Univ. of Tokyo — Perovskite-type oxides ABO_3 have been widely studied for its dielectricity. The properties of these materials significantly change by substituting A or B cations, while compositions of A and B cations are limited to (A^{2+}, B^{4+}) and (A^{3+}, B^{3+}) for charge neutrality. Recently, it has been demonstrated that oxygen anions in $BaTiO_3$ can be partially substituted with hydride ions (H^-)[2], suggesting that more varieties of compositions might be realized (e.g., (A^+, B^{4+})) combined with oxygen substitution. In this work, using first-principles calculations, we investigate an unsynthesized model composition with the oxygen substitution, $KTi(O_2H)$. This compound is expected to crystalize into the perovskite-type structure from its tolerance factor. We confirm its stability with the crystal structure optimization and calculation of its formation energy for possible reactions. The material is insulating with large electronic polarization and has two-dimensional low-energy electronic states within Ti–O–H planes. For its unconventional composition and the peculiar two-dimensional property, this material may realize novel electronic properties.

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[2]Y. Kobayashi *et. al.*, Nature Mater. **11**, 507 (2012).

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