Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-principles predictions of perovskite-type alkali metal titanium oxyhydrides with two-dimensional electronic states NOBUYA SATO, RYOSUKE AKASHI, Dept. of Phys., Univ. of Tokyo, SHINJI TSUNEYUKI, Dept. of Phys., Univ. of Tokyo and ISSP, Univ. of Tokyo — The electric properties of perovskite-type oxides ABO_3 can be controlled by substituting A and B cations, while their chemical compositions are limited by the charge neutrality, e.g., $A^{2+}B^{4+}O_3^{2-}$. A way of realizing other compositions is substitution of oxygen atoms with monovalent anions, e.g., $A^{+}B^{4+}O_2^{2-}X^{-}$. Such substitution has been recently realized in experiments with fluorine atoms[1], and more recently, with hydrogen[2]. Since the valence orbital character of hydrogen atoms (s) is different from that of oxygen and fluorine atoms (p), oxyhydrides should exhibit interesting electronic properties. In this study, we explore the property of unsynthesized oxyhydrides $ATiO_2H$ for alkali metals A by first-principles calculations[3]. For A = K, Rb, Cs, two-dimensional electronic states emerge at the valence band maximum, which has H 1s characteristics. Their dielectric and piezoelectric properties are also discussed.

[1]T. Katsumata et al., J. Appl. Phys. 104, 044101 (2008).
[2]Y. Kobayashi *et al.*, Nature Mater. **11**, 507 (2012)
[3]For A = K, N. Sato and S. Tsuneyuki, Appl. Phys. Lett. **109**, 172903 (2016).

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Date submitted: 10 Nov 2016 Electronic form version 1.4