格子欠陥マルチフェロイクスとその力学的機能制御に関する第一原理解析

First-principles Study of Lattice-defect Multiferroics and Strain Engineering

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Multiferroics in nanoscale dimensions are promising for novel functional device paradigms, such as magnetoelectric memory, due to intriguing cross-coupling between coexisting ferroelectric and (anti-)ferromagnetic order parameters. However, the ferroic order is inevitably destroyed below the critical dimension of several nanometers. Here, we demonstrate a new path toward realization of ultimately small multiferroics while resolving the controversial origin of dilute ferromagnetism that unexpectedly emerges in nanoparticles of nonmagnetic ferroelectric $PbTiO_3$. Systematic exploration using state-of-the-art hybrid Hartree-Fock density functional calculations[1] as well as the DFT+U calculations with a theoretical Hubbard U derived from the constrained random phase approximation (cRPA) successfully identifies that oxygen vacancies formed at surfaces/grain boundaries induce (anti-)ferromagnetism due to local non-stoichiometry and orbital symmetry breaking [2]. The localized character of emerged magnetization allows an individual oxygen vacancy to act as an atomic-scale multiferroic object with a nonlinear magnetoelectric effect that involves rich FM-AFM-NM phase transitions in response to switching spontaneous polarization. Moreover, we also demonstrate that the local (anti-)ferromagnetism can emerge at dislocations as a line defect. Therefore, defects in ferroelectric oxides can behaver as atomic-scale low-dimensional multiferroics. Engineering these multiferroic features opens a new avenue to the design of ultrahigh-density integration for atomic-scale multiferroics [3].

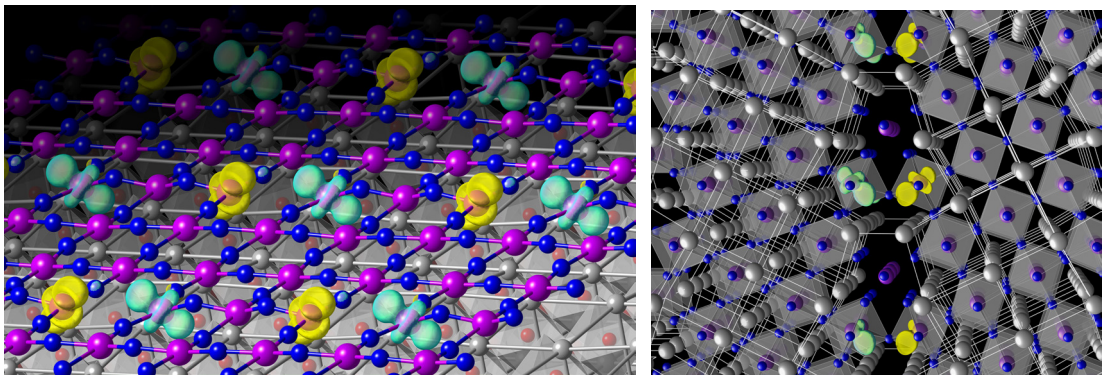

Figure. Vacancy-induced magnetism at ferroelectric $PbTiO_3$ surface(left) and grain boundary(right).

References:

[1] T.Shimada, et al., Phys. Rev. B, 87, 174111 (2013).

[2] T.Shimada, et al., Nano Letters, 15, 27-33 (2015); T.Shimada, et al., Phys. Rev. Lett., 115, 107202 (2015); T. Xu, T. Shimada, et al., Nano Letters, 16, 454-458 (2016).

[3] T. Xu, T. Shimada, et al, Phys. Rev. B 92, 104106 (2015).