First principles of antiferroelectric solar container

Can antiferroelectricity be used in nanoelectromechanical systems?
This work demonstrates the anisotropic phase transition mechanism and ideal antiferroelectricity with large digital electrostrain in antiferroelectric thin films,offering a new avenue for applications of antiferroelectricity in nanoelectromechanical systems.

Why is antiferroelectricity important?
The first attribute of antiferroelectricity is the ability to be switched from a nonpolar state to a polar state by electric field below the breakdown strength of the material, giving rise to the emblematic double hysteresis loop.

Can antiferroelectrics be used for energy storage and conversion applications?
Herein, we provide perspectives on the development of antiferroelectrics for energy storage and conversion applications, as well as a comprehensive understanding of the structural origin of antiferroelectricity and field-induced phase transitions, followed by design strategies for new lead-free antiferroelectrics.

When was antiferroelectricity invented?
The notion of antiferroelectricity dates back to the early 1950s,and the formal definition of an antiferroelectric (AFE) state was proposed by Kittel in 1951based on the antiferromagnetism scheme .

Does antiferroelectricity exist?
Apart from the conventional perovskite- and fluorite-type oxides,antiferroelectricity was reported to existin a wide range of unconventional structures as well,which highly broadened the AFE family and understanding of antiferroelectricity.

What are the characteristics of antiferroelectric materials?
Antiferroelectric materials show phase transition characteristicssuch as electric field,temperature,and pressure in the presence of an external field that leads to tremendous electrical properties (Chao et al.,2020).

The famous triple-well potential of antiferroelectric PbZrO3 is modified in the nanocapacitor limit in such a way as to swap the positions of the global and local minima, stabilizing ...

Niranjan, First principle study of lead free piezoelectric AgNbO3 and (Ag1-xKx)NbO3 solid solutions, Solid State Commun., No 152, ?. 1707 DOI: 10.1016/j.ssc.2012.05.002 Moriwake, First-principles ...

First-principles calculations indicate that inhibiting oxygen vacancy formation raises the bandgap from 1.41 to 2.45 eV, thereby enhancing structural stability and breakdown strength. Guided ...

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Antiferroelectric materials are defined as substances that exhibit a transition from an antiferroelectric state to a ferroelectric state under high electric fields, which enhances their dielectric properties and ...

First-principles study of competing ferroelectric and antiferroelectric instabilities in BaTiO 3 / BaO superlattices Eric Bousquet 1,2, Javier Junquera 3, and Philippe Ghosez 1

We first give a brief overview of first-principles electronic structure calculations. We emphasize the aspects of first-principles calculations relevant to the study of magnetoelectric and ...

Bandgap engineering and antiferroelectric stability of tantalum doped silver niobate ceramics from first-principles Yonghao Xu a, Minyuan Zhan a, Danyang Zhang a, Feng Shi a, ...

La doped $ {mathrm {SrFeO}}_ {3}$, $ {mathrm {La}}_ {1/3} {mathrm {Sr}}_ {2/3} {mathrm {FeO}}_ {3}$, exhibits a metal-to-insulator transition accompanied by both antiferromagnetic ...

Antiferroelectric (AFE) materials are of great interest owing to their scientific rich-ness and their utility in high- energy density capacitors. Here, the history of AFEs is reviewed, and the characteristics of ...

In this theoretical study, we have systematically investigated the electronic, structural, and chemical bonding properties of AgNb1-xTaxO3 (x = 0.00, 0.125, 0.25, 0.375, 0.50, abbreviated ...

The application of Sodium niobate (NaNbO3, NN) ceramics with antiferroelectric (AFE) crystal phase faces the severe limitations in low energy density and efficiency due to the instability of the ...

Herein, we report through first-principles calculations that the single-layer ?-AlOOH exhibits intrinsic ferroelectric (FE), antiferroelectric (AFE), and ferroelastic properties.

This work demonstrates the anisotropic phase transition mechanism and ideal antiferroelectricity with large digital electrostrain in antiferroelectric thin films, offering a new avenue ...

Here we present a first-principles investigation to that end.Main modes and their couplings.-We followed the usual first-principles approach to the investigation of a non-reconstructive phase transition, taking ...

A new NaNbO 3 -based composition, namely (1- x)NaNbO 3 -xSrSnO 3, was designed with a combination of first-principles calculations and experimental characterization.

The antiferroelectric Pbcm phase of silver niobate (AgNbO3) has received increasing attention owing to its environmental safety (as it is lead-free), compatibility, and superior energy-storage density ...

The first attribute of antiferroelectricity is the ability to be switched from a nonpolar state to a polar state by

electric field below the breakdown strength of the material, giving rise to the ...

In2013, Bunnette et al. [13,14] used first-principles method to predict a new class of antiferroelectric materials by proposing about 70 compounds that were classified as follow: 37 ...

re are many more antiferroelectric compounds to be discovered. In this Rapid Communication, we use first-principles calculations to provide clear evidence that the tetragonal phase of ZrO2 is an ...

We employ first-principles calculations to investigate the ferroelectric properties and the bulk photovoltaic effect (BPVE) of antimony sulfur iodide (SbSI). The BPVE enables direct ...

In this review, we will concentrate on the recent development and applications of phase field model and first-principles-derived effective Hamiltonian method in the study of ECE in ...

Density functional calculations are performed to investigate the experimentally-reported field-induced phase transition in thin-film ZrO2 (J. Muller et al., Nano. Lett. 12, 4318). We find a small ...

First-principle-based calculations of full phonon dispersion, including but not limited to perovskites and their derivatives, can be very helpful in identifying phonon modes and AFE structures.

Ceramics International, volume 50, issue 8, pages 13459-13466 Bandgap engineering and antiferroelectric stability of tantalum doped silver niobate ceramics from first-principles Yonghao Xu 1, ...