First principles of antiferroelectric energy storage

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.

Is antiferroelectricity a resurgence in energy-efficient applications?
As a close relative of ferroelectricity,antiferroelectricity has received a recent resurgence of interestdriven by technological aspirations in energy-efficient applications,such as energy storage capacitors,solid-state cooling devices,explosive energy conversion,and displacement transducers.

What are antiferroelectric materials used for?
Antiferroelectric materials exhibit a unique electric-field-induced phase transition,which enables their use in energy storage,electrocaloric cooling,and nonvolatile memory applications. However...

Can antiferroelectric materials store energy in pulsed-power technologies?
The polarization response of antiferroelectrics to electric fields is such that the materials can store large energy densities,which makes them promising candidatesfor energy storage applications in pulsed-power technologies. However,relatively few materials of this kind are known.

Are antiferroelectrics a promising material with high energy density?
Continued efforts are being devoted to find materials with high energy density,and antiferroelectrics (AFEs) are promisingbecause of their characteristic polarization-electric field (P - E) double hysteresis loops schematized in Fig. 1a (ref. 4).

Are antiferroelectric materials irreversible?
Antiferroelectric materials exhibit a unique electric-field-induced phase transition,which enables their use in energy storage,electrocaloric cooling,and nonvolatile memory applications. However,in many prototype antiferroelectrics this transition is irreversible,which prevents their implementation.

Sm-doping induced large enhancement of antiferroelectric and energy storage performances of (111) oriented PbZrO 3 thin films. Ceram. Int., 45 (17) (2019), pp. 23586-23591. ... Antiferroelectricity in thin-film ZrO 2 from first principles. Phys. Rev. B, 90 (14) (2014), Article 140103. Crossref View in Scopus Google Scholar

In this work, we demonstrate a general approach to promote the reversibility of this phase transition by targeted modification of the material''s local structure. A new NaNbO 3-based composition,...

As a paradigm of engineering antiferroelectric (AFE)-ferroelectric (FE) transition on rare-Earth/titanium complex oxides by solid solution to develop advanced dielectric energy storage materials with high energy

density and ...

First-principles investigations of elastic properties and energetics of antiferroelectric and ferroelectric phases of PbZrO 3 ... {mathrm{PbZrO}}_{3}$ is regarded as the first antiferroelectric and currently is under intense reexamination. ... Antiferroelectrics have been recently sparking interest due to their potential use in energy storage ...

First-Principle calculations of the ferroelectric properties of the La doped Silver Niobate. A significant improvement in ferroelectric polarization (from 1.9 to 14.86 mC/cm2) was ...

In this study, we investigate the energy storage performance of AFR by building a phase field model of a doped AFE system. In the model, both the local phase transition ...

A new generation of environmentally benign NaNbO 3 (NN)-based antiferroelectric ceramics have gained great interest in energy storage capacitors. Nevertheless, the low breakdown electric field (E b) and high energy density loss in pure NN ceramic restrict the improvement of the energy storage property.A combined optimization strategy was ...

Specifically, using high-throughput second-principles calculations, we engineer PbTiO 3 /SrTiO 3 superlattices to optimize their energy storage performance at room temperature (to maximize density and release efficiency) ...

Here, we present a review of recent applications of first principles and first-principles-based effective Hamiltonian approaches to the study of energy storage in ferroelectrics,...

Antiferroelectricity of NaNbO3: Single-crystal experimental study and first-principles ... Similar to the canonical antiferroelectric (AFE) compound PbZrO 3 in Pb(Zr,Ti)O 3 solid-solutions, the presence of double hysteresis loops and that of electric field-induced phase transitions are important characteristics of NaNbO 3 AFE materials; yet the phase transition behavior in the ...

Reversible field-induced phase transitions define antiferroelectric perovskite oxides and lay the foundation for high-energy storage density materials, required for future green technologies.

Designing lead-free antiferroelectrics for energy storage . Antiferroelectric capacitors hold great promise for high-power energy storage. Here, through a first-principles-based computational ...

Energy storage has become a crucial research topic. Dielectric capacitors play a significant role in the energy storage system and pulse power devices due to their ultra-fast charge discharge rates, high power density, and safety advantages. However, their energy storage density is inferior to that of batteries and electrochemical supercapacitors.

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In recent years, high performance energy storage technologies and devices have attracted tremendous research in academia and industry, influenced by the growing demand for electrical energy and excessive consumption of conventional energy sources in current society [1], [2], [3].Up to date, based on the redox reactions (like lithium batteries, fuel cells and super ...

Extensive research has been conducted on silver niobite (AgNbO 3)-based antiferroelectric ceramics for their promising applications in energy storage applications, with various compositional modifications explored to improve their energy storage capabilities this theoretical study, we have systematically investigated the electronic, structural, and chemical ...

Antiferroelectric materials exhibit a unique electric-field-induced phase transition, which enables their use in energy storage, electrocaloric cooling, and nonvolatile memory applications. However, in many prototype antiferroelectrics this transition is irreversible, which prevents their implementation.

Antiferroelectrics (AFEs) are promising candidates in energy-storage capacitors, electrocaloric solid-cooling, and displacement transducers. As an actively studied lead-free antiferroelectric (AFE ...

The NaNbO 3 antiferroelectrics have been considered as a potential candidate for dielectric capacitors applications. However, the high-electric-field-unstable antiferroelectric phase resulted in low energy storage density and efficiency. Herein, good energy storage properties were realized in (1-x)NaNbO 3-xNaTaO 3 ceramics, by building a new phase boundary.

First-principles-based simulations have been used previously to explain the size-driven transition into ferroelectric phase 16. It was proposed that the presence of the surface favors the ...

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. For instance, high-throughput first-principles calculations revealed a class of antiferroelectric materials in the orthorhombic MgSrSi structure type ...

Design of Lead-Free Antiferroelectric (1 - x)NaNbO 3 -xSrSnO 3 Compositions Guided by First-Principles Calculations ... Antiferroelectric materials exhibit a unique electric-field-induced phase transition, which enables their use in energy storage, electrocaloric cooling, and nonvolatile memory applications.

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 ...

The exploration of two-dimensional (2D) ferroic materials and the investigation of ferroic couplings are highly desired in view of the design of next-generation functional devices. Herein, we report through first-principles

calculations that the single-layer ensuremath{gamma}-AlOOH exhibits intrinsic ferroelectric (FE), antiferroelectric (AFE), and ferroelastic properties. ...

Bandgap engineering and antiferroelectric stability of tantalum doped silver niobate ceramics from first-principles ... -based antiferroelectric ceramics for their promising applications in energy storage. Various compositional modifications have been In ...

PbZrO3 has been broadly considered as a prototypical antiferroelectric material for high-power energy storage. A recent theoretical study suggests that the ground state of PbZrO3 is threefold ...

Nonvolatile random access memory and energy storage based on antiferroelectric like hysteresis in ZrO 2. Adv Funct Mater, 26 (41) (2016), pp. 7486-7494. Crossref View in Scopus Google Scholar ... Antiferroelectricity in thin-film ZrO 2 from first principles. Phys Rev B, 90 (14) (2014), Article 140103. Crossref View in Scopus Google Scholar

We have studied ab initio the phase transition in ${mathrm{PbZrO}}_{3}$, a perovskite oxide usually presented as the prototypic antiferroelectric material. Our work reveals the crucial role that antiferrodistortive modes---involving concerted rotations of the oxygen octahedra in the structure---play in the transformation, as they select the observed ...

Electrochemical batteries, thermal batteries, and electrochemical capacitors are widely used for powering autonomous electrical systems [1, 2], however, these energy storage devices do not meet output voltage and current requirements for some applications.Ferroelectric materials are a type of nonlinear dielectrics [[3], [4], [5]].Unlike batteries and electrochemical ...

With the rapid development of economic and information technology, the challenges related to energy consumption and environmental pollution have recen...

The antiferroelectric Pbcm phase of silver niobate (AgNbO 3) has received increasing attention owing to its environmental safety (as it is lead-free), compatibility, and superior energy-storage density compared with its ferroelectric counterparts. We comprehensively investigated the effects of La doping at Ag sites (i.e., Ag 0.88 La 0.12 NbO 3) on the structural, ...

Antiferroelectric materials are promising for diverse applications ranging from energy harvesting 1 and solid state cooling devices 2 over electromechanical transducers 3 to energy storage ...

Antiferroelectric materials are attractive for energy storage applications and are becoming increasingly important for power electronics. Lead-free silver niobate (AgNbO 3) and sodium niobate (NaNbO 3) antiferroelectric ceramics have ...

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