The two-day workshop on Analytical Ferroelectrics and Nanoscale

DTU Energy, Building 301, Room 101

10th and 11th June 2024

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Day one: June 10th
DTU Energy
Building 301, room 101

9:00-10:30:
Prof. Long-Qing Chen
Thermodynamics and Phase-field Method of Nanoscale Ferroelectric Polarization Patterns: Part 1

11:00-12:30:
Prof. Anna Morozovska (online)
Analytical Description of Size Effects and Strain Engineering of Low-Dimensional Ferroelectric Materials

Day two: June 11th
DTU Energy
Building 301, room 101

9:00-10:30:
Prof. Long-Qing Chen
Thermodynamics and Phase-field Method of Nanoscale Ferroelectric Polarization Patterns: Part 2

11:00-12:30:
Prof. Anna Morozovska (online)
Ferri-ionic Coupling in CuInP2S6 Nanoflakes: High and Low Polarization States and Controllable Negative Capacitance

Ministry of Higher Education and Science
Danish Agency for Science and Higher Education

DTU Energy
Department for Energy
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Abstracts

Thermodynamics and Phase-field Method of Nanoscale Ferroelectric Polarization Patterns

Long-Qing Chen
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The presentation discusses the thermodynamic stability of ferroelectric polarization distributions in nanoscale heterostructures. It will start with introducing the fundamental equation of thermodynamics for homogeneous ferroelectric crystals connecting the classical thermodynamics and Landau description of ferroelectric instability. It will then be followed by the discussion on the thermodynamics and phase-field method of inhomogeneous ferroelectric crystals containing domain structures involving long-range elastic and electrostatic interactions and domain wall energy. The focus will be on the thermodynamic stability and the size effect of nanoscale ferroelectric polarization patterns based on phase-field simulations of ferroelectric heterostructures under different mechanical and electrostatic boundary conditions.

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Anna N. Morozovska

Analytical Description of Size Effects and Strain Engineering of Low-Dimensional Ferroelectric Materials

The lecture is devoted to the analytical methods based on the Landau-Ginzburg-Devonshire approach and variational principle, which allow the analytical description of size effects and strain engineering of low-dimensional ferroelectric materials, such as thin films and small nanoparticles. It will start with the introduction of the experimental evidence of the size-induced and strain-induced transitions and related phenomena in the low-dimensional ferroelectric materials. Next, we introduce the fundamentals of the Landau-Ginzburg-Devonshire approach combined with the classical electrostatics and elasticity theory, and variational principle for the description of size-induced and strain-induced effects in ferroelectric thin films and small nanoparticles. The focus will be on the comparison with experimental results and finite element modelling, as well as on the theoretical predictions of the size- and strain-control of polar and piezoelectric properties of low-dimensional ferroelectric materials.

Ferri-ionic Coupling in CuInP2S6 Nanoflakes: High and Low Polarization States and Controllable Negative Capacitance*

We consider nanoflakes of van der Waals ferrielectric CuInP2S6 covered by an ionic surface charge and reveal the appearance of polar states with relatively high polarization ~ 5 µC/cm2 and stored free charge ~ 10 µC/cm2, which can mimic "mid-gap" states related with a surface field-induced transfer of Cu and/or In ions in the van der Waals gap. The change in the ionic screening degree and mismatch strains induce a broad range of the transitions between paraelectric phase, antiferroelectric, ferrielectric, and ferroelectric-like states in CuInP2S6 nanoflakes. We predict that the CuInP2S6 nanoflakes reveal features of the controllable negative capacitance effect, which make them attractive for advanced electronic devices, such as nano-capacitors and gate oxide nanomaterials with reduced heat dissipation.

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