FLAIR Colloquium

Tuesday, 8. May 2025, 16:00
Room R77, Building L2|01

Zoom-Link

Charge carriers at ferroelectric domain walls in bismuth ferrite

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Abstract

Ferroelectrics are materials with a spontaneous electric polarization, whose direction is not necessarily uniform, but forms domains with different orientations, similar to magnetic domains. The ferroelectric domains either form spontaneously, or they can be created intentionally. The interfaces between the domains, the ferroelectric domain walls, can add new functionality to the host crystal. For example, in lead zirconate titanate or bismuth ferrite, which are normally insulating or semiconducting, ferroelectric domain walls act as electrically conducting planes [1,2].

Additional point defects can further influence the behavior of the domain walls. In my talk I will speak about atomic defects and charge carriers at ferroelectric domain walls in bismuth ferrite, and how they could be detected in optical spectra, according to ab initio calculations. I will present evidence that excess electrons in bismuth ferrite form strongly localized small polaron states at ferroelectric domain walls, where they can either recombine with holes under emission of photoluminescence with photon energies below the band gap energy or participate in electronic transport by thermally activated hopping of small electron polarons.

[1] J. Guyonnet, I. Gaponenko, S. Gariglio, and P. Paruch, Conduction at domain walls in insulating $Pb(Zr_{0.2}Ti_{0.8})O_3$ thin films, Adv. Mater. 23, 5377 (2011).
[2] J. Seidel, L. W. Martin, Q. He, et al., Conduction at domain walls in oxide multiferroics, Nat. Mater. 8, 229 (2009).