TRR 80 Seminar

Am Dienstag, den 8. Januar um 16:00 Uhr

spricht

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über das Thema

Defects at epitaxial interfaces and domain walls in ferroelectric oxides

Epitaxial strain has enabled exploration and tuning of the properties of oxide thin films. While it was initially presumed that coherent epitaxial strain was mitigated by altering bond lengths and angles, the last five years there has been increasing awareness of point defects as a strain relaxation mechanism. This can be regarded as inverse “chemical expansion”, which is a widely studied phenomenon in the solid state ionics community. Here we investigate the complex interplay between strain, oxygen vacancies and ferroic properties in 100-strained AMnO3 where A is Ca2+, Sr2+ or Ba2+.
Understanding the domain wall (DW) mobility in ferroelectrics is key to controlling and fine-tune the domain structure and hence the ferroelectric properties. Similarly, controlling the DW conductivity is enabling knowledge for developing DW-based nanoscale circuitry. The DW mobility and conductivity strongly couples to the defect chemistry of the material. Aliovalent dopants and oxygen defects can modify the charge carrier concentration and act as pinning centers. The overall aim of this study is to obtain chemical guidelines from first principles calculations for how to control the DW mobility and conductivity through defect chemistry. The improper ferroelectric YMnO3 has a complex and exotic DW structure, including both neutral and charged head-to-head and tail-to-tail DWs as well as topologically protected vortex cores. YMnO3 displays great chemical flexibility, where donor and acceptor doping of both cation sublattices as well as both oxygen deficiency and excess is possible. This makes the hexagonal manganites an ideal model system for studying the interplay between point defects and DW properties. Using DFT calculations, we investigate differences in DW mobility in the presence and absence of aliovalent dopants on both cation sublattices. We extend this investigation to include mobile oxygen vacancies and interstitials, before comparing with available experimental data on hexagonal manganites.

Gäste sind herzlich willkommen.
Der Vortrag findet im Seminarraum S-288, Institut für Physik,
Universität Augsburg statt.

Gastgeber: Dr. Stephan Krohns
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