



# TRR 80 Seminar

Am Dienstag, den 12. Juli um 16:00 Uhr

spricht

## Prof. Dr. Derek C. Sinclair

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über das Thema

### *A combined experimental and computational study into the composition-property relationships of rare earth and Ca-doped BaTiO<sub>3</sub> ceramic*

Alkaline and Rare earth ions are often used to chemically dope ferroelectric BaTiO<sub>3</sub> to modify its electrical properties for commercial applications such as positive temperature coefficient of resistance (ptcr) thermistors and multilayer capacitors (MLC's); however, in many cases the role(s) of the dopants are poorly understood. In part, this is because some dope only onto the Ba- or Ti- site whereas others dope onto both sites (self compensation) and in many cases ionic and/or electronic charge compensation mechanisms are required to maintain electroneutrality. Here we present results from a recent computer simulation study and a systematic phase diagram-impedance spectroscopy study for a range of RE<sup>3+</sup> ions, including La<sup>3+</sup>, Nd<sup>3+</sup>, Gd<sup>3+</sup> and Yb<sup>3+</sup> and for Ca<sup>2+</sup>. We highlight; (i) the influence of RE ion size on the doping mechanism(s) and the rich variety of electrical properties displayed, including n-type, p-type or intrinsic conduction and ferroelectric relaxor behaviour dependent on the composition; (ii) the influence and usefulness of cation variance (strain) in A-site (isovalent) Ca-doped materials for developing the next generation (X8R) of MLC's; (iii) an alternative explanation for the so-called 'Donor (La) doping' mechanism for semiconductivity based on oxygen-loss as opposed to direct electronic compensation; and (iv) the unexpected but remarkable properties of B-site (acceptor) Ca-doped materials including reversible ferroelectric domain switching with remanent polarization,  $P_r \sim 0 \text{ Ccm}^2$  (double P-E hysteresis loops) and significant nonlinear recoverable electrostrain at room temperature to novel field-enhanced bulk conductivity at elevated temperatures ( $\sim 150 - 600 \text{ }^\circ\text{C}$ ) that may be associated with ionization of underbonded oxide ions adjacent to Ca acceptor dopants.

The overall aim of the seminar is to highlight the rich defect chemistry and functionality of ferroelectric BaTiO<sub>3</sub> and that despite being discovered in the 1940's and heavily exploited in oxide-based electronic components since the 1960's we still have much to learn about this particular perovskite.

Gäste sind herzlich willkommen.

Der Vortrag findet im Seminarraum S-288/ Physikgebäude Süd, Universität Augsburg statt.

Gastgeber: Dr. Stephan Krohns

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