

# SFB 608

## Einladung zum Kolloquium

**Ort:** Universität zu Köln  
II. Physikalisches Institut, Seminarraum 201

**Zeit:** 27. Juni 2007, 14:30 Uhr

**Sprecher:** J.P. Itié,  
Synchrotron SOLEIL

**Thema:** High pressure phase transformation  
ferroelectric perovskites: the local point of  
view

The Ti K edge X-ray absorption has been measured under high pressure at room temperature for  $\text{ATiO}_3$  perovskites (A= Ca, Sr, Ba and Pb). All these compounds have strong pre-edge features related to the local environment of the Ti atom. The intensity of these features depends on the off centre position of the Ti atom and is modified under high pressure. For  $\text{CaTiO}_3$ <sup>1</sup>, which is not ferroelectric at room pressure, no change occurs under pressure. In the case of  $\text{SrTiO}_3$ <sup>2</sup>, the antiferrodistorsive instability appears above 5 GPa. At the same pressure a slight decrease of the intensity of the pre-edge feature occurs, indicating that the Ti was not at the centre of the oxygen octahedron under ambient conditions. The ferroelectric local instability decreases when pressure is increased ( $\text{PbTiO}_3$ <sup>1</sup>) and eventually vanishes at high pressure ( $\text{BaTiO}_3$ <sup>3</sup>). The results on  $\text{BaTiO}_3$  have been confirmed by x-ray diffraction on single crystals where a disappearance of the diffuse scattering lines is observed above 10 GPa

- 1 A.C. Dhaussy, N. Jaouen, J.P. Itié, A. Rogalev, S. Marinel and A. Veres, Pressure induced phase transition in  $\text{PbTiO}_3$  studied by x-ray absorption spectroscopy at the Ti K edge, Proceeding of SRI 2006 28 May-2 June 2006, Daegu, Korea
- 2 D. Cabaret, B. Couzinet, A.M. Flank, J.P. Itié, P. Lagarde and A. Polian, Ti K pre-edge in  $\text{SrTiO}_3$  under pressure: experiments and full-potential first principles calculations, AIP Conference Proceedings Volume **882** X-RAY ABSORPTION FINE STRUCTURE - XAFS13: 13th International Conference, Stanford, California (USA), 9-14 July 2006, p 120
- 3 J.P. Itié, B. Couzinet, A. Polian, A.M. Flank and P. Lagarde, Pressure-induced disappearance of the local rhombohedral distortion in  $\text{BaTiO}_3$ , Europhys. Lett. **74**, 706 (2006)

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