

Gemeinsames Kolloquium der Sonderforschungsbereiche 445, 491 und 616

Vortragender: **Dr. R. I. Eglitis**

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Gast von Prof. Entel

Thema: ***Ab initio* calculations of SrTiO₃, BaTiO₃, PbTiO₃, CaTiO₃, BaZrO₃, SrZrO₃ and PbZrO₃ (001) and (011) surfaces as well as Nb impurity segregation towards the SrTiO₃ surface**

Abstract:

While the (001) surfaces of ABO₃ perovskites, such as SrTiO₃, BaTiO₃, PbTiO₃, CaTiO₃, SrZrO₃, PbZrO₃ and BaZrO₃ have been extensively studied [1-5], much less is known about the (011) surfaces. On the (001) surfaces, I consider both AO (A=Sr, Ba, Pb or Ca) and BO₂ (B=Ti or Zr) terminations. The (001) surface AO layer is found to relax inward for all seven materials with the sole exception of SrO-terminated SrTiO₃ (001) surface first layer O atom.

My calculated surface rumpplings of 6.77 % for the SrO-terminated SrZrO₃ (001) and 3.32 % for the PbO-terminated PbZrO₃ (001) surfaces are almost ten times larger than those of the corresponding ZrO₂-terminated SrZrO₃ and PbZrO₃ (001) surfaces [5].

As for the (011) surfaces, I consider three types of surfaces, terminating on a BO layer, A layer and O layer. Turning now to the surface energies, I find that both the AO and BO₂-terminated (001) surfaces are about equally energetically favorable and may co-exist. In contrast, I see very large differences in the surface energies on the ABO₃ (011) surfaces. I demonstrate that Nb is a shallow donor in SrTiO₃ and discuss also its segregation towards the SrTiO₃ surface [6].

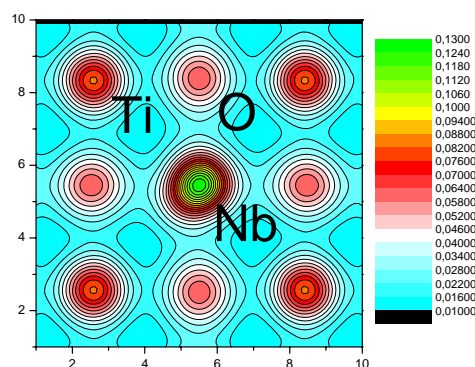


Fig. 1 Total charge density map for Nb doped SrTiO₃ calculated by means of hybrid B3PW method.

- References
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 6. R. I. Eglitis and E. A. Kotomin, Physica B **405**, 3164 (2010).

Zeit: ***Dienstag*, 12. Juli 2011, 12:00 Uhr** (Sondertermin)

Ort: **Gebäude MD, Raum 349** (Campus Duisburg)
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Interessenten sind herzlich willkommen

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